

3/14/05 10/765,227d.

text search

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005

=> filcaplus

FILCAPLUS IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list-of-commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (=>).

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907--14-Mar 2005 VOL 142 ISS 12

FILE LAST UPDATED: 13 Mar 2005 (20050313/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s  $\beta$ (w) carbolin?

1304215 BETA

1328 BETAS

1304286 B

(BETA OR BETAS)

5148 CARBOLIN?

L1

4000 B(W) CARBOLIN?

=> s 3-hydroxamic(w)acid

6245340 3

6448 HYDROXAMIC

29 3-HYDROXAMIC

(3(W) HYDROXAMIC)

3949235 ACID

1468030 ACIDS

4425180 ACID

(ACID OR ACIDS)

L2

28 3-HYDROXAMIC(W)ACID

=> del L2  
DELETE L2? (Y)/N:y

=> s 3-hydroxamic(3a)acid  
6245340 3  
6448 HYDROXAMIC  
29 3-HYDROXAMIC  
(3(W)HYDROXAMIC)  
3949235 ACID  
1468030 ACIDS  
4425180 ACID  
(ACID OR ACIDS)  
L2 29 3-HYDROXAMIC(3A)ACID

=> s L1 and L2  
L3 0 L1 AND L2

=> d cost  
COST IN U.S. DOLLARS

CONNECT CHARGES  
NETWORK CHARGES  
SEARCH CHARGES

SINCE FILE	TOTAL
ENTRY	SESSION
1.95	2.10
0.30	0.36
15.12	15.12
-----	-----
17.37	17.58

FULL ESTIMATED COST

IN FILE 'CAPLUS' AT 16:50:57 ON 14 MAR 2005

=> s pyrido(4a)indol?  
9255 PYRIDO  
97256 INDOL?  
L4 2431 PYRIDO(4A)INDOL?

=> s L2 and L4  
L5 0 L2 AND L4

=> s carboxamide  
14666 CARBOXAMIDE  
4151 CARBOXAMIDES  
L6 17060 CARBOXAMIDE  
(CARBOXAMIDE OR CARBOXAMIDES)

=> s L1 and L6  
L7 108 L1 AND L6

=> s rauwolfia  
1536 RAUWOLFIA  
4 RAUWOLFIAS  
L8 1536 RAUWOLFIA  
(RAUWOLFIA OR RAUWOLFIAS)

=> s norharmane  
116 NORHARMANE  
1 NORHARMANES  
L9 117 NORHARMANE  
(NORHARMANE OR NORHARMANES)

=> s L1 or L8 or L9  
L10 5567 L1 OR L8 OR L9

=> d L10

L10 ANSWER 1 OF 5567 CAPLUS COPYRIGHT 2005 ACS on STN  
AN 2005:219323 CAPLUS  
TI Variability of ribosomal RNA genes in **Rauwolfia** species:  
parallelism between tissue culture-induced rearrangements and interspecies  
polymorphism  
AU Andreev, I. O.; Spiridonova, K. V.; Solovyan, V. T.; Kunakh, V. A.  
CS Institute of Molecular Biology and Genetics, Academy Zabolotnogo Street,  
National Academy of Science of Ukraine, 150, Kiev-143, 03143, Ukraine  
SO Cell Biology International (2005), 29(1), 21-27  
CODEN: CBIIEV; ISSN: 1065-6995  
PB Elsevier B.V.  
DT Journal  
LA English

=> del L10  
DELETE L10? (Y)/N:y

=> s L1 or L4 or L8 or L9  
L10 7516 L1 OR L4 OR L8 OR L9

=> d his

(FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005)

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

L1 4000 S B(W) CARBOLIN?  
L2 29 S 3-HYDROXAMIC (3A) ACID  
L3 0 S L1 AND L2  
L4 2431 S PYRIDO (4A) INDOL?  
L5 0 S L2 AND L4  
L6 17060 S CARBOXAMIDE  
L7 108 S L1 AND L6  
L8 1536 S RAUWOLFIA  
L9 117 S NORHARMANE  
L10 7516 S L1 OR L4 OR L8 OR L9

=> s "hydroxamic acid" or carboxamide  
6448 "HYDROXAMIC"  
3949235 "ACID"  
1468030 "ACIDS"  
4425180 "ACID"  
("ACID" OR "ACIDS")  
6225 "HYDROXAMIC ACID"  
("HYDROXAMIC" (W) "ACID")  
14666 CARBOXAMIDE  
4151 CARBOXAMIDES  
17060 CARBOXAMIDE  
(CARBOXAMIDE OR CARBOXAMIDES)  
L11 23223 "HYDROXAMIC ACID" OR CARBOXAMIDE

=> s L10 and L11  
L12 148 L10 AND L11

=> s "carboxylic acid" (4a) hydroxy (3a) amide  
225341 "CARBOXYLIC"  
46 "CARBOXYLICS"  
225359 "CARBOXYLIC"  
("CARBOXYLIC" OR "CARBOXYLICS")  
3949235 "ACID"  
1468030 "ACIDS"  
4425180 "ACID"

("ACID" OR "ACIDS")  
207462 "CARBOXYLIC ACID"  
("CARBOXYLIC"(W)"ACID")  
422026 HYDROXY  
9 HYDROXIES  
422035 HYDROXY  
(HYDROXY OR HYDROXIES)  
118181 AMIDE  
74816 AMIDES  
161241 AMIDE

(AMIDE OR AMIDES)  
L13 143 "CARBOXYLIC ACID"(4A)HYDROXY(3A)AMIDE

=> s L11 or L13

L14 23352 L11 OR L13

=> s L10 and L14

L15 149 L10 AND L14

=> d his

(FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005)

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

L1 4000 S B(W)CARBOLIN?  
L2 29 S 3-HYDROXAMIC(3A)ACID  
L3 0 S L1 AND L2  
L4 2431 S PYRIDO(4A)INDOL?  
L5 0 S L2 AND L4  
L6 17060 S CARBOXAMIDE  
L7 108 S L1 AND L6  
L8 1536 S RAUWOLFIA  
L9 117 S NORHARMANE  
L10 7516 S L1 OR L4 OR L8 OR L9  
L11 23223 S "HYDROXAMIC ACID" OR CARBOXAMIDE  
L12 148 S L10 AND L11  
L13 143 S "CARBOXYLIC ACID"(4A)HYDROXY(3A)AMIDE  
L14 23352 S L11 OR L13  
L15 149 S L10 AND L14

=> s L15 not L12

L16 1 L15 NOT L12

=> d L16

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:511094 CAPLUS

DN 139:85365

TI Preparation of pyrrolopyrimidine A2b selective antagonist compounds,  
method of synthesis and therapeutic use

IN Castelhana, Arlindo L.; Mckibben, Bryan; Steinig, Arno G.

PA Osi Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 223 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053361	A2	20030703	WO 2002-US40890	20021220
	WO 2003053361	A3	20031224		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,  
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 US 2003229067 A1 20031211 US 2002-326005 20021220  
 EP 1467995 A2 20041020 EP 2002-805644 20021220  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK  
 PRAI US 2001-343443P P 20011220  
 WO 2002-US40890 W 20021220  
 OS CASREACT 139:85365; MARPAT 139:85365

=> d his

(FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005)

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

L1 4000 S B(W) CARBOLIN?  
 L2 29 S 3-HYDROXAMIC(3A) ACID  
 L3 0 S L1 AND L2  
 L4 2431 S PYRIDO(4A) INDOL?  
 L5 0 S L2 AND L4  
 L6 17060 S CARBOXAMIDE  
 L7 108 S L1 AND L6  
 L8 1536 S RAUWOLFIA  
 L9 117 S NORHARMANE  
 L10 7516 S L1 OR L4 OR L8 OR L9  
 L11 23223 S "HYDROXAMIC ACID" OR CARBOXAMIDE  
 L12 148 S L10 AND L11  
 L13 143 S "CARBOXYLIC ACID"(4A) HYDROXY(3A) AMIDE  
 L14 23352 S L11 OR L13  
 L15 149 S L10 AND L14  
 L16 1 S L15 NOT L12

=> d L15 ibib abs

L15 ANSWER 1 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:105517 CAPLUS

TITLE: Anxiogenic properties of an inverse agonist selective  
 for  $\alpha 3$  subunit-containing GABAA receptors

AUTHOR(S): Atack, John R.; Hutson, Peter H.; Collinson, Neil;  
 Marshall, George; Bentley, Graham; Moyes, Christopher;  
 Cook, Susan M.; Collins, Ian; Wafford, Keith;  
 McKernan, Ruth M.; Dawson, Gerard R.

CORPORATE SOURCE: Neuroscience Research Centre, Merck Sharp & Dohme  
 Research Laboratories, Harlow, CM20 2QR, UK

SOURCE: British Journal of Pharmacology (2005), 144(3),  
 357-366

CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

LANGUAGE: English

AB  $\alpha 3$ IA (6-(4-pyridyl)-5-(4-methoxyphenyl)-3-carbomethoxy-1-methyl-1H-  
 pyridin-2-one) is a pyridone with higher binding and functional affinity  
 and greater inverse agonist efficacy for GABAA receptors containing an  
 $\alpha 3$  rather than an  $\alpha 1$ ,  $\alpha 2$  or  $\alpha 5$  subunit. If doses  
 are selected that minimise the occupancy at these latter subtypes, then  
 the in vivo effects of  $\alpha 3$ IA are most probably mediated by the

DOCUMENT NUMBER: 141:207055  
 TITLE: Preparation of  $\beta$ -carboline hydroxamic acids as HIV-integrase inhibitors  
 INVENTOR(S): Kuki, Atsuo; Li, Xinqiang; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu  
 PATENT ASSIGNEE(S): Pfizer Inc., USA  
 SOURCE: PCT Int. Appl., 57 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

(our app.)

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067531	A1	20040812	WO 2004-IB259	20040123
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
PRIORITY APPLN. INFO.:			US 2003-443223P	P 20030127
OTHER SOURCE(S):			MARPAT 141:207055	
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB **Beta-carboline hydroxamic acid**  
 compds. Title compds. I and II [wherein R1, R2, R3, R4, R5, R6 = independently H, halo, alkoxy/alkyl, alkenyl, alkynyl, OH and derivs., NO2, NH2 and derivs.; R7 = (un)substituted alk(en/yn)yl; R8, R9 = independently H, (un)substituted alk(en/yn)yl; X = (CR10R11)n; R10, R11 = independently H, halo, OH and derivs., NH and derivs., (un)substituted lower alk(en/yn)yl; n = 1-3; their pharmaceutically acceptable salts and solvates] were prepared as inhibitors or modulators the activity of HIV-integrase enzyme. Examples include 13 synthetic prepns., bioassays for HIV-integrase activity and HIV-1 cell protection. For example, III was prepared, in 39% yield, from Et 9H-3-carboline-3-carboxylate, 4-fluorobenzyl bromide and NH2OH. Selected I and II displayed IC50 values in the range of 0.234 - 0.713  $\mu$ M for the inhibition of HIV-integrase. Thus, I and II are useful for treating HIV-integrase-mediated diseases and conditions (no data).

TI Preparation of  $\beta$ -carboline hydroxamic acids as HIV-integrase inhibitors

AB **Beta-carboline hydroxamic acid**  
 compds. Title compds. I and II [wherein R1, R2, R3, R4, R5, R6 = independently H, halo, alkoxy/alkyl, alkenyl, alkynyl, OH and derivs., NO2, NH2 and derivs.; R7 = (un)substituted alk(en/yn)yl; R8, R9 = independently H, (un)substituted alk(en/yn)yl; X = (CR10R11)n; R10, R11 = independently H, halo, OH and derivs., NH and derivs., (un)substituted lower alk(en/yn)yl; n = 1-3; their pharmaceutically acceptable salts and solvates] were prepared as inhibitors or modulators the activity of HIV-integrase enzyme. Examples include 13 synthetic prepns., bioassays for HIV-integrase activity and HIV-1 cell protection. For example, III was prepared, in 39% yield, from Et 9H-3-carboline-3-carboxylate, 4-fluorobenzyl bromide and NH2OH. Selected I and II displayed IC50 values in the range of 0.234 - 0.713  $\mu$ M for the inhibition of HIV-integrase.

Thus, I and II are useful for treating HIV-integrase-mediated diseases and conditions (no data).

- ST carboline **hydroxamic acid** prepn HIV integrase inhibitor AIDS
- IT Anti-AIDS agents  
Antiviral agents.  
Human  
(preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT Drug delivery systems  
(prodrugs; preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT Radiochemical analysis  
(receptor-binding; preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT AIDS (disease).  
Human immunodeficiency virus  
(treatment; preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT 737817-45-7P 737817-46-8P 737817-47-9P, 9-(4-Fluorobenzyl)-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide  
737817-48-0P, 9-[(5-Chlorothien-2-yl)methyl]-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-49-1P,  
9-(3-Chloro-2-fluorobenzyl)-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-50-4P,  
9-Benzyl-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-51-5P, 9-(4-Methylbenzyl)-N-Hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-52-6P,  
9-(2,4-Difluorobenzyl)-N-hydroxy-9H-3-carboline-3-carboxamide 737817-53-7P, 9-(3-Chloro-2,6-difluorobenzyl)-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-56-0P,  
6-Amino-9-(3-chlorobenzyl)-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-59-3P, 9-(3-Chloro-2,6-difluorobenzyl)-N-hydroxy-N-methyl-9H- $\beta$  -carboline-3-carboxamide 737817-60-6P, N-Benzyl-9-(3-chloro-2,6-difluorobenzyl)-N-hydroxy-9H- $\beta$  -carboline-3-carboxamide 737817-61-7P, 9-(4-Fluorobenzyl)-N-hydroxy-N-methyl-9H- $\beta$  -carboline-3-carboxamide  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(HIV-inhibitor; preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT 737817-54-8P, Ethyl 9-(3-chloro-2,6-difluorobenzyl)-9H- $\beta$  -carboline-3-carboxylate 737817-55-9P 737817-57-1P, Ethyl 9-(3-chlorobenzyl)-6-nitro-9H- $\beta$  -carboline-3-carboxylate 737817-58-2P, Ethyl 6-amino-9-(3-chlorobenzyl)-9H- $\beta$  -carboline-3-carboxylate  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT 52350-85-3, HIV integrase  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(of HIV, inhibition; preparation of  $\beta$  -carboline **hydroxamic acids** as HIV-integrase inhibitors)
- IT 104-81-4, 4-Methylbenzyl bromide 459-46-1, 4-Fluorobenzyl bromide 620-20-2, 3-Chlorobenzyl chloride 622-30-0, O-Benzylhydroxyamine 23784-96-5, 2-Chloro-5-(chloromethyl)thiophene 23915-07-3, 2,4-Difluorobenzyl bromide 74214-62-3, Ethyl 9H- $\beta$  -carboline-3-carboxylate 78539-50-1, Ethyl 6-nitro-9H- $\beta$  -carboline-3-carboxylate 85070-47-9, 3-Chloro-2-fluorobenzyl bromide 261762-47-4, 3-Chloro-2,6-difluorobenzyl

bromide 737817-62-8, Ethyl 9-(4-fluorobenzyl)-9H- $\beta$ -  
**carboline-3-carboxylate**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of  $\beta$ -**carboline hydroxamic acids** as HIV-integrase inhibitors)

IT 740984-68-3 740984-69-4 740984-70-7 740984-71-8

RL: PRP (Properties)  
(unclaimed nucleotide sequence; preparation of  $\beta$ -  
**carboline hydroxamic acids** as HIV-integrase inhibitors)

L15 ANSWER 9 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:633526 CAPLUS

DOCUMENT NUMBER: 141:167817

TITLE: Treatment of diseases with alpha-7 NACH receptor full agonists

INVENTOR(S): Groppi, Vincent Edward, Jr.; Rogers, Bruce Nelsen;  
Rudmann, Daniel Gregory

PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA

SOURCE: PCT Int. Appl., 142 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004064836	A2	20040805	WO 2004-IB115	20040112
WO 2004064836	A3	20041223		
W:	AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ			

PRIORITY APPLN. INFO.: US 2003-441801P P 20030122

OTHER SOURCE(S): MARPAT 141:167817

AB The present invention relates to compositions and methods to treat diseases or conditions with alpha-7 nicotinic acetylcholine receptor (AChR) full agonists by decreasing levels of tumor necrosis factor-alpha and/or by stimulating vascular angiogenesis.

IT 272-23-1P, Thieno[2,3-b]pyridine 704-91-6P, 1H-Indazole-6-carboxylic acid 1073-31-0P, 3,4-Thiophenedicarboxaldehyde 1074-99-3P, 2,4-Dimethyl-5-nitropyridine 1851-22-5P, 3-Chloropyridine 1-oxide 4442-54-0P, 2,3-Dihydro-1,4-benzodioxine-6-carboxylic acid 5832-38-2P, 2-Formyl-4-methyl-5-nitropyridine 6624-49-3P, 3-Isoquinolinecarboxylic acid 7040-07-5P, Furan-2,3-dicarboxaldehyde 7137-33-9P, Benzo[b]thiophene-2,3-dicarboxaldehyde 13452-14-7P 14757-78-9P 15112-41-1P, 1,3-Benzoxazole-5-carboxylic acid 18853-32-2P, 3,4-Dicyanothiophene 19005-93-7P, 1H-Indole-2-carboxaldehyde 21344-31-0P, Thieno[2,3-b]pyridine-5-carbonitrile 21472-88-8P, Ethyl 5-hydroxy-6-oxo-1,2,3,6-tetrahydropyridine-4-carboxylate 21473-14-3P 21473-16-5P, exo-1-Azabicyclo[2.2.1]heptan-3-ol 21492-03-5P, cis-4-(Hydroxymethyl)piperidin-3-ol 23680-40-2P, Methyl 3-bromopropiolate 24621-70-3P, 1H-Indole-2-methanol 25557-50-0P, Thieno[2,3-b]pyridine-7-oxide 28872-85-7P, 2-(3-Bromo-2-furyl)-1,3-dioxolane 34668-25-2P, Ethyl furo[2,3-b]pyridine-2-carboxylate 34668-26-3P, Furo[2,3-b]pyridine-2-carboxylic acid 35350-37-9P 36404-88-3P, 2-Chloronicotinaldehyde 38180-46-0P, 3-Chloropyridine-2-carbonitrile 40789-79-5P, 2-(Benzoyloxy)-1-nitroethane 56538-57-9P, [[(Benzoyloxy)carbonyl]amino](hydroxy)acetic acid 58123-77-6P,



carboxylic acid hydrochloride 588720-16-5P, 6-Bromopyrrolo[1,2-c]pyrimidine-3-carboxylic acid hydrochloride 588720-29-0P, Imidazo[1,5-a]pyridine-7-carboxylic acid 588720-48-3P, Pyrrolo[1,2-a]pyrazine-3-carboxylic acid hydrochloride 588720-59-6P, Pyrazino[1,2-a]indole-3-carboxylic acid hydrochloride 655785-32-3P, Phenyl 4-iodo-1H-pyrazole-1-carboxylate 655785-40-3P, 4-Nitrophenyl 4-(2-chlorophenyl)-1H-pyrazole-1-carboxylate 711082-67-6P 711083-82-8P, (3S)-3-(Phenoxymethyl)-2,3-dihydro-1,4-benzodioxine-6-carboxylic acid 711084-61-6P, Oxazolo[4,5-c]pyridine-6-carboxylic acid 711084-89-8P 711085-20-0P 711085-34-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of azabicycloalkane derivs. useful as  $\alpha 7$  nAChR agonists)

IT 473795-11-8P 473795-39-0P, endo-1-Azabicyclo[3.2.1]octan-3-amine dihydrochloride 478148-80-0P 478148-90-2P 478149-24-5P 478149-31-4P 478149-43-8P 478149-45-0P 478149-46-1P, N-(1-Azabicyclo[2.2.2]oct-3-yl) furo[2,3-c]pyridine-5-carboxamide 478149-53-0P 478149-55-2P 478149-58-5P 478149-67-6P 478149-68-7P 478149-71-2P 478149-73-4P 478149-74-5P 478149-78-9P 478149-83-6P 478149-95-0P 478149-96-1P 478150-02-6P 478152-73-7P 478152-78-2P 478155-32-7P 478169-41-4P 478169-43-6P 478169-45-8P 478169-49-2P 478169-75-4P 478169-89-0P 478170-28-4P 500556-90-1P 501892-52-0P 501893-00-1P 501893-01-2P 501893-02-3P 501893-03-4P 501893-10-3P 501893-13-6P 501893-17-0P 501893-18-1P 501893-19-2P 501893-20-5P 501893-23-8P 501897-07-0P 501901-29-7P 501901-30-0P 501901-33-3P 501901-43-5P 501901-52-6P 508201-60-3P 508201-72-7P 508201-75-0P 508201-78-3P 508201-88-5P 508201-93-2P 508202-02-6P 508202-05-9P 508202-22-0P 508202-68-4P 508203-04-1P 508203-63-2P 521277-79-2P 521278-10-4P 521278-18-2P 527680-56-4P 527681-36-3P 527681-66-9P 588702-81-2P 588702-84-5P 588702-87-8P 588703-09-7P 588703-11-1P 588703-26-8P 588703-34-8P 588703-38-2P 588703-46-2P 588703-51-9P 588704-11-4P 588705-34-4P 588705-35-5P 588705-36-6P 588705-41-3P 588705-43-5P 588705-51-5P 588705-52-6P 588705-80-0P 588720-18-7P 588720-21-2P 588720-37-0P 588720-43-8P 588720-45-0P 588720-54-1P 588720-56-3P 588720-60-9P 588720-69-8P 588723-76-6P 588726-61-8P 588726-81-2P 590369-66-7P 590369-67-8P 590369-75-8P 590370-28-8P 590370-30-2P 590370-42-6P 655785-29-8P 655785-31-2P 655785-35-6P 655785-43-6P 711085-63-1P 711085-68-6P 711085-92-6P 711086-35-0P 711086-40-7P 711086-65-6P 711086-78-1P 711088-12-9P 711089-23-5P 711089-83-7P 711089-98-4P 711090-06-1P 711090-20-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azabicycloalkane derivs. useful as  $\alpha 7$  nAChR agonists)

L15 ANSWER 14 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:453214 CAPLUS

DOCUMENT NUMBER: 141:23513

TITLE: Preparation of substituted **pyrido**[3,2-b]**indoles** for use in pharmaceutical compositions for the treatment of HIV-infection

INVENTOR(S): Kesteleyn, Bart Rudolf Romanie; Van De Vreken, Wim; Kindermans, Natalie Maria Francisca; Canard, Maxime Francis Jean-Marie Ghislain; Hertogs, Kurt; Bettens, Eva; De Vroey Veronique, Corine Paul; Jochmans, Dirk Edward Desire

PATENT ASSIGNEE(S): Tibotec Pharmaceuticals Ltd., Ire.

SOURCE: PCT Int. Appl., 91 pp.

CODEN: PIXXD2

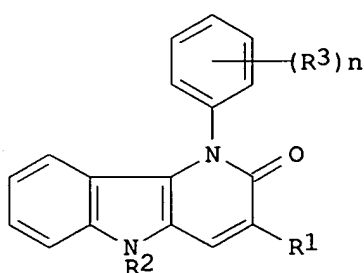
DOCUMENT TYPE: Patent

LANGUAGE: English

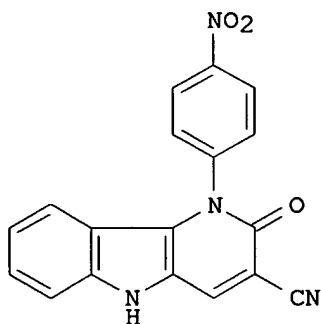
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046143	A1	20040603	WO 2003-EP50837	20031114
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			EP 2002-79783	A 20021115
			US 2002-434950P	P 20021220
OTHER SOURCE(S):		MARPAT 141:23513		
GI				



I



II

- AB **Pyrido[3,2-b]indoles**, such as I [R1 = H, CN, halogen, **carboxamide**, carboxyl, etc.; R2 = H, alkyl, alkenyl, cycloalkyl, heterocyclyl, heterocyclylalkyl, etc.; R3 = NO2, CN, NH2, OH, CO2H, CONH2, methanimidamidyl, alkoxy, acyl, etc.; n = 1, 2, 3], were prepared for therapeutic use and anti-HIV agents. Thus, **pyrido[3,2-b]indole** II was prepared via a five step synthetic scheme starting from 1-acetyl-3-hydroxyindole, 4-nitroaniline and Et cyanoacetate. The prepared **pyrido[3,2-b]indoles** were tested for inhibition of HIV reverse transcriptase, for metabolism using human liver microsomal fractions and for anti-HIV activity.
- TI Preparation of substituted **pyrido[3,2-b]indoles** for use in pharmaceutical compositions for the treatment of HIV-infection
- AB **Pyrido[3,2-b]indoles**, such as I [R1 = H, CN, halogen, **carboxamide**, carboxyl, etc.; R2 = H, alkyl, alkenyl, cycloalkyl, heterocyclyl, heterocyclylalkyl, etc.; R3 = NO2, CN, NH2, OH, CO2H, CONH2, methanimidamidyl, alkoxy, acyl, etc.; n = 1, 2, 3], were prepared for therapeutic use and anti-HIV agents. Thus, **pyrido[3,2-b]indole** II was prepared via a five step synthetic scheme starting from 1-acetyl-3-hydroxyindole, 4-nitroaniline and Et cyanoacetate. The prepared **pyrido[3,2-b]indoles** were tested for inhibition of HIV reverse transcriptase, for metabolism using human liver microsomal fractions and for anti-HIV activity.
- IT Anti-AIDS agents  
Human  
(preparation of substituted **pyrido[3,2-b]indoles** for use in pharmaceutical compns. for the treatment of HIV-infection)
- IT Drug delivery systems  
(prodrugs; preparation of substituted **pyrido[3,2-b]indoles**)

for use in pharmaceutical compns. for the treatment of HIV-infection)

IT AIDS (disease)  
(treatment; preparation of substituted **pyrido**[3,2-b]  
**indoles** for use in pharmaceutical compns. for the treatment of  
HIV-infection)

IT 9068-38-6  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(HIV, inhibitors; preparation of substituted **pyrido**[3,2-b]  
**indoles** for use in pharmaceutical compns. for the treatment of  
HIV-infection)

IT 304465-35-8P 352548-47-1P 698396-45-1P 698396-64-4P 698396-65-5P  
698396-80-4P 698396-93-9P 698396-97-3P 698396-98-4P 698397-05-6P  
698397-11-4P 698397-15-8P 698397-18-1P 698397-19-2P 698397-25-0P  
698397-41-0P 698397-43-2P 698397-44-3P 698397-45-4P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic  
preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of substituted **pyrido**[3,2-b]**indoles** for use  
in pharmaceutical compns. for the treatment of HIV-infection)

IT 698397-13-6  
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use);  
BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)  
(preparation of substituted **pyrido**[3,2-b]**indoles** for use  
in pharmaceutical compns. for the treatment of HIV-infection)

IT 698396-30-4P 698396-31-5P 698396-32-6P 698396-33-7P 698396-34-8P  
698396-35-9P 698396-36-0P 698396-37-1P 698396-38-2P 698396-39-3P  
698396-40-6P 698396-41-7P 698396-42-8P 698396-43-9P 698396-44-0P  
698396-46-2P 698396-47-3P 698396-48-4P 698396-49-5P 698396-50-8P  
698396-51-9P 698396-52-0P 698396-53-1P 698396-54-2P 698396-55-3P  
698396-56-4P 698396-57-5P 698396-58-6P 698396-59-7P 698396-60-0P  
698396-61-1P 698396-62-2P 698396-63-3P 698396-66-6P 698396-67-7P  
698396-68-8P 698396-69-9P 698396-70-2P 698396-71-3P 698396-72-4P  
698396-73-5P 698396-74-6P 698396-75-7P 698396-76-8P 698396-77-9P  
698396-78-0P 698396-79-1P 698396-81-5P 698396-82-6P 698396-83-7P  
698396-84-8P 698396-85-9P 698396-86-0P 698396-87-1P 698396-88-2P  
698396-89-3P 698396-90-6P 698396-91-7P 698396-92-8P 698396-94-0P  
698396-95-1P 698396-96-2P 698396-99-5P 698397-00-1P 698397-01-2P  
698397-02-3P 698397-03-4P 698397-04-5P 698397-06-7P 698397-07-8P  
698397-08-9P 698397-09-0P 698397-10-3P 698397-12-5P 698397-14-7P  
698397-16-9P 698397-17-0P 698397-20-5P 698397-21-6P 698397-22-7P  
698397-23-8P 698397-24-9P 698397-26-1P 698397-27-2P 698397-28-3P  
698397-29-4P 698397-30-7P 698397-31-8P 698397-32-9P 698397-33-0P  
698397-34-1P 698397-35-2P 698397-36-3P 698397-37-4P 698397-38-5P  
698397-39-6P 698397-40-9P 698397-42-1P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)  
(preparation of substituted **pyrido**[3,2-b]**indoles** for use  
in pharmaceutical compns. for the treatment of HIV-infection)

IT 62-55-5, Thioacetamide 79-04-9, Chloroacetyl chloride 94-05-3  
100-01-6, 4-Nitroaniline, reactions 104-94-9, 4-Methoxyaniline  
105-56-6, Ethyl cyanoacetate 106-40-1, 4-Bromoaniline 108-59-8,  
Dimethyl malonate 109-01-3, 1-Methylpiperazine 109-70-6,  
1-Bromo-3-chloropropane 123-75-1, Pyrrolidine, reactions 530-62-1,  
1,1'-Carbonyldiimidazole 628-36-4, N,N'-Diformylhydrazine 696-59-3,  
2,5-Dimethoxytetrahydrofuran 703-80-0, 3-Acetylintole 873-74-5,  
4-Aminobenzonitrile 4637-24-5 4755-77-5, Ethyl oxalyl chloride  
5050-41-9, 1-(2-Chloroethyl)pyrrolidine 5292-43-3, tert-Butyl  
bromoacetate 6160-65-2, 1,1'-Thiocarbonyldiimidazole 13331-23-2,  
2-Furylboronic acid 16800-68-3 33025-60-4, 1-Acetyl-3-hydroxyindole  
39931-77-6, Ethyl 3-pyridylacetate 55552-70-0, 3-Furylboronic acid  
149104-90-5, 4-Acetylphenylboronic acid  
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of substituted **pyrido**[3,2-**b**]indoles for use  
in pharmaceutical compns. for the treatment of HIV-infection)  
IT 14757-68-7P 19012-02-3P 52971-32-1P 67766-00-1P 85729-26-6P  
136429-63-5P 167954-14-5P 167954-19-0P 304465-28-9P 658041-31-7P  
698397-46-5P 698397-47-6P 698397-48-7P 698397-49-8P 698397-50-1P  
698397-51-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of substituted **pyrido**[3,2-**b**]indoles for use  
in pharmaceutical compns. for the treatment of HIV-infection)

L15 ANSWER 15 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:414634 CAPLUS

DOCUMENT NUMBER: 140:423661

TITLE: Preparation of substituted 1,8-naphthyridines as  
anti-infective agents

INVENTOR(S): Pratt, John K.; Betebenner, David A.; Donner, Pamela  
L.; Green, Brian E.; Kempf, Dale J.; McDaniel, Keith  
F.; Maring, Clarence J.; Stoll, Vincent S.; Zhang,  
Rong

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 91 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004097492	A1	20040520	US 2002-285714	20021101
US 2004087577	A1	20040506	US 2003-410853	20030410
US 2004162285	A1	20040819	US 2003-625121	20030723
WO 2004041818	A1	20040521	WO 2003-US34707	20031031
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			US 2002-285714	A2 20021101
			US 2003-410853	A2 20030410
			US 2003-625121	A 20030723
			US 2003-679881	A 20031006

OTHER SOURCE(S): MARPAT 140:423661

GI

LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:111299  
 AB Minisci-type radical carbamoylation of 1-bromo- $\beta$  -  
**carboline** (I) gives the 3-substituted product in low yield,  
 whereas 1-acetyl- $\beta$  -**carboline** (II) reacts under  
 ipso-substitution of the acetyl group. Cyanations of the N-oxides of I  
 and II occur under clean ipso-substitution of the groups in 1-position.  
 1-Me derivs. show no tendency to react under ipso-substitution.  
 REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT  
 TI Unexpected ipso-substitutions at the  $\beta$  -**carboline**  
 nucleus  
 AB Minisci-type radical carbamoylation of 1-bromo- $\beta$  -  
**carboline** (I) gives the 3-substituted product in low yield,  
 whereas 1-acetyl- $\beta$  -**carboline** (II) reacts under  
 ipso-substitution of the acetyl group. Cyanations of the N-oxides of I  
 and II occur under clean ipso-substitution of the groups in 1-position.  
 1-Me derivs. show no tendency to react under ipso-substitution.  
 IT Carbamoylation  
 Substitution reaction  
 (carbamoylation of  $\beta$  -**carbolines** via  
 ipso-substitution)  
 IT 244-63-3,  $\beta$  -**Carboline** 2506-09-4, 1-Methyl-  
 $\beta$  -**carboline** 2-oxide 50892-83-6, 1-Acetyl-  
 $\beta$  -**carboline** 159898-15-4, 1-Bromo- $\beta$   
**-carboline**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (carbamoylation of  $\beta$  -**carbolines** via  
 ipso-substitution)  
 IT 24223-07-2P,  $\beta$  -**Carboline** 2-oxide 647825-14-7P,  
 1-Acetyl- $\beta$  -**carboline** 2-oxide 647825-15-8P,  
 1-Bromo- $\beta$  -**carboline** 2-oxide  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (carbamoylation of  $\beta$  -**carbolines** via  
 ipso-substitution)  
 IT 38940-60-2P,  $\beta$  -**Carboline**-1-**carboxamide**  
 79960-43-3P,  $\beta$  -**Carboline**-1-carbonitrile  
 93138-03-5P, 1-Methyl- $\beta$  -**carboline**-3-carbonitrile  
 647825-13-6P, 1-Bromo- $\beta$  -**carboline**-3-  
**carboxamide** 647825-16-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (carbamoylation of  $\beta$  -**carbolines** via  
 ipso-substitution)

=> ind patents

FILE 'ENCOMPAT2' ACCESS NOT AUTHORIZED

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
110.09	110.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-15.33	-15.33

CA SUBSCRIBER PRICE

INDEX 'CAOLD, CAPLUS, CASREACT, CROPU, DGENE, DPCI, ENCOMPAT, EPFULL,  
 FRANCEPAT, FRFULL, FSTA, IFIPAT, IMSPATENTS, INPADOC, JAPIO, KOREAPAT,  
 LITALERT, NTIS, PAPERCHEM2, PATDD, PATDPA, PATDPAFULL, PCTFULL, PCTGEN,  
 PIRA, PROUSDDR, PS, RAPRA, RDISCLOSURE, ...'

ENTERED AT 17:00:01 ON 14 MAR 2005

37 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view  
search error messages that display as 0\* with SET DETAIL OFF.

=> s L15

149 FILE CAPLUS  
20 FILE CASREACT  
4 FILE DGENE  
5 FILES SEARCHED...  
3 FILE DPCI  
1 FILE ENCOMPPAT  
216 FILE EPFULL  
2 FILE FRANCEPAT  
11 FILE FRFULL  
68 FILE IFIPAT  
12 FILES SEARCHED...  
24 FILE INPADOC  
1 FILE JAPIO  
1 FILE KOREAPAT  
2 FILE NTIS  
7 FILE PATDPAFULL  
22 FILES SEARCHED...  
251 FILE PCTFULL  
60 FILE PROUSDDR  
26 FILES SEARCHED...  
5 FILE SYNTHLINE  
839 FILE USPATFULL  
33 FILES SEARCHED...  
108 FILE USPAT2  
16 FILE WPIDS  
35 FILES SEARCHED...  
16 FILE WPINDEX

21 FILES HAVE ONE OR MORE ANSWERS, 37 FILES SEARCHED IN STNINDEX

L17 QUE L15

=> d rank

F1 839 USPATFULL  
F2 251 PCTFULL  
F3 216 EPFULL  
F4 149 CAPLUS  
F5 108 USPAT2  
F6 68 IFIPAT  
F7 60 PROUSDDR  
F8 24 INPADOC  
F9 20 CASREACT  
F10 16 WPIDS  
F11 16 WPINDEX  
F12 11 FRFULL  
F13 7 PATDPAFULL  
F14 5 SYNTHLINE  
F15 4 DGENE  
F16 3 DPCI  
F17 2 FRANCEPAT  
F18 2 NTIS  
F19 1 ENCOMPPAT  
F20 1 JAPIO  
F21 1 KOREAPAT

=> fil ifipat  
COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST	ENTRY 4.13	SESSION 114.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-15.33

FILE 'IFIPAT' ENTERED AT 17:04:06 ON 14 MAR 2005  
COPYRIGHT (C) 2005 IFI CLAIMS(R) Patent Services (IFI)

FILE COVERS 1950 TO PATENT PUBLICATION DATE: 10 Mar 2005 (20050310/PD)  
FILE LAST UPDATED: 11 Mar 2005 (20050311/ED)  
HIGHEST GRANTED PATENT NUMBER: US2005033839  
HIGHEST APPLICATION PUBLICATION-NUMBER: US2005055750  
UNITERM INDEXING IS AVAILABLE IN THE IFIUIDB FILE  
UNITERM INDEXING LAST UPDATED: 10 Feb 2005 (20050210/UP)  
INDEXING CURRENT THROUGH PAT PUB DATE: 27 Jul 2004 (20040727/PD)

INCL, INCLM, INCLS fields added. Please refer to ONLINE News for details.

=> s L15

84243 BETA  
67 BETAS  
84276 B  
(BETA OR BETAS)  
461 CARBOLIN?  
328 B(W) CARBOLIN?  
2283 PYRIDO  
17729 INDOL?  
491 PYRIDO (4A) INDOL?  
64 RAUWOLFIA  
1 NORHARMANE  
1121 "HYDROXAMIC"  
440812 "ACID"  
117319 "ACIDS"  
463571 "ACID"  
( "ACID" OR "ACIDS" )  
1073 "HYDROXAMIC ACID"  
( "HYDROXAMIC" (W) "ACID" )  
5210 CARBOXAMIDE  
1147 CARBOXAMIDES  
5853 CARBOXAMIDE  
(CARBOXAMIDE OR CARBOXAMIDES)  
68634 "CARBOXYLIC"  
4 "CARBOXYLICS"  
68636 "CARBOXYLIC"  
( "CARBOXYLIC" OR "CARBOXYLICS" )  
440812 "ACID"  
117319 "ACIDS"  
463571 "ACID"  
( "ACID" OR "ACIDS" )  
62583 "CARBOXYLIC ACID"  
( "CARBOXYLIC" (W) "ACID" )  
98293 HYDROXY  
7 HYDROXIES  
98297 HYDROXY  
(HYDROXY OR HYDROXIES)  
33672 AMIDE  
14465 AMIDES  
43627 AMIDE  
(AMIDE OR AMIDES)  
332 "CARBOXYLIC ACID" (4A) HYDROXY (3A) AMIDE

L18

68 L10 AND L14

=&gt; d L18 50-68-ibib-abs kwic

L18 ANSWER 50 OF 68 IFIPAT COPYRIGHT 2005 IFI on STN  
AN 03337016 IFIPAT;IFIUDB;IFICDB  
TITLE: 1H-PYRIDO(3,4-B)INDOLE-4-CARBOXAMIDE DERIVATIVES, PREPARATION AND APPLICATION THEREOF IN THERAPEUTICS  
INVENTOR(S): Evanno; Yannick, Bullion, FR  
George; Pascal, Saint Arnoult en Yvelines, FR  
Legalloudec; Odette, Morigny, FR  
Maloizel; Christian, Meudon, FR  
Sevrin; Mireille, Paris, FR  
PATENT ASSIGNEE(S): Synthelabo, Le Plessis Robinson, FR  
PRIMARY EXAMINER: Powers, Fiona T  
AGENT: Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P.

	NUMBER	PK	DATE
PATENT INFORMATION:	US 6075021	A	20000613
	(CITED IN 001 LATER PATENTS)		
	WO 9815552		19980416
APPLICATION INFORMATION:	US 1999-284070		19990407
	WO 1997-FR1750		19971008
			19990407 PCT 371 date
			19990407 PCT 102(e) date
EXPIRATION DATE:	8 Oct 2017		

	NUMBER	DATE
PRIORITY APPLN. INFO.:	FR 1996-12229	19961008
FAMILY INFORMATION:	US 6075021	20000613
DOCUMENT TYPE:	Utility	
	CERTIFICATE OF CORRECTION	
CORRECTION DATE:	30 Apr 2002	
FILE SEGMENT:	CHEMICAL	
	GRANTED	

MICROFILM REEL NO: 010431 FRAME NO: 0614  
010441 0399  
010762 0343

NUMBER OF CLAIMS: 15  
AB Compounds of general formula (I)

# FIG-01

in which the variables are as defined in the specification, their preparation and their application in therapeutics.

CLMN 15

TI 1H-PYRIDO(3,4-B)INDOLE-4-CARBOXAMIDE  
DERIVATIVES, PREPARATION AND APPLICATION THEREOF IN THERAPEUTICS  
ECLM 1. A compound having general formula (I)

1-(O=), 2-R2, 3, 4-(=), 4-(R3-N(-R4)-CO-), 9-R1, X- (I)  
2, 3, 4, 9-TETRAHYDRO-1H-PYRIDO(3,4-b)INDOLE

in which X represents a hydrogen or halogen atom or a (C1 -C3) alkyl, (C1 -C3)alkoxy, trifluoromethyl or. . .

L18 ANSWER 51 OF 68 IFIPAT COPYRIGHT 2005 IFI on STN  
AN 03327564 IFIPAT;IFIUDB;IFICDB



R4, RA and R9 each are hydrogen; and that R4, RA and R9 each is not hydrogen when X is oxygen and R3 is OCH3. have valuable pharmacological properties.

CLMN 15

TI **BETA-CARBOLIN-3-CARBOXYLIC ACID DERIVATIVES USEFUL FOR TREATING ANXIETY AND RELATED DISORDERS; TRANQUILIZERS**

AB A **Beta -carbolin-3-carboxylic acid derivative of the formula**

#### D R A W I N G

wherein: X is oxygen, . . .

ECLM 1. A **Beta -carbolin-3-carboxylic acid derivative of the formula**

3-(R3-C(=X)-), 4-R4, RA, 9-R9-**BETA-CARBOLINE**

wherein: X is oxygen, sulphur or NR10, wherein R10 is hydrogen or alkyl; R3 is NR11R12, wherein R11. . .

ACLM 2. A **Beta -carbolin-3-carboxylic acid derivative of claim 1, wherein the A-ring has 1-2 RA's.**

3. N-methyl- **Beta -carbolin-3-carboxamide.**

4. N',N'-(dimethyl)- **Beta -carbolin-3-hydrazide, a compound of claim 1.**

10. A **Beta -carbolin-3-carboxylic acid derivative of the formula**

#### D R A W I N G

wherein: X is oxygen, . . .

11. A **Beta -carbolin-3-carboxylic acid derivative of claim 10, wherein R11 and R12 together with the connecting nitrogen atom form pyrrolidine, piperidine, 3-methoxycarbonylpiperidine, 4-hydroxy-3-ethoxycarbonylpiperidine, . . .**

12. A **Beta -carbolin-3-carboxylic acid derivative of claim 10, wherein X is oxygen.**

13. A **Beta -carbolin-3-carboxylic acid derivative of claim 1, wherein X is oxygen.**

14. A **Beta -carbolin-3-carboxylic acid derivative of claim 1, wherein at least one of R11 and R12 is amino optionally substituted with C1-10-alkyl.**

15. A **Beta -carbolin-3-carboxylic acid derivative of claim 1, wherein R11 and R12 together with the connecting nitrogen atom form pyrrolidine, piperidine, piperidine-3-methoxycarbonyl, piperidine-4-hydroxy-3-ethoxycarbonyl, . . .**

L18 ANSWER 66 OF 68 IFIPAT COPYRIGHT 2005 IFI on STN

AN 02075054 IFIPAT;IFIUDB;IFICDB

TITLE: **H-PYRIDO(2,3-B)INDOLE**

**-3-CARBOXYLIC ACID ESTER COMPOUNDS HAVING USEFUL PHARMACEUTICAL ACTIVITY; TREATMENT OF PROPHYLAXIS OF ANXIETY OR DEPRESSION**

INVENTOR(S):

Forbes, Ian T, Harlow, GB

Thompson, Mervyn, Harlow, GB

PATENT ASSIGNEE(S):

Beecham Group plc, Brentford, GB

PRIMARY EXAMINER:

Lee, Mary C

ASSISTANT EXAMINER:

Davis, Zinna Northington

AGENT:

Barr, David K

Evans, Emily A

Haley, Jr, James F

NUMBER

PK

DATE

PATENT INFORMATION: US 4952584 A 19900828  
 (CITED IN 009 LATER PATENTS)  
 APPLICATION INFORMATION: US 1989-307068 19890206  
 EXPIRATION DATE: 28 Aug 2007

	APPLN. NUMBER	DATE	GRANTED PATENT NO. OR STATUS
CONTINUATION-IN-PART OF:	US 1987-1589	19870109	ABANDONED

	NUMBER	DATE
PRIORITY APPLN. INFO.:	GB 1986-651	19860111
	GB 1989-383	19890119
FAMILY INFORMATION:	US 4952584	19900828
DOCUMENT TYPE:	Utility	
	EXPIRED	
FILE SEGMENT:	CHEMICAL	
	GRANTED	
OTHER SOURCE:	CA 114:122347	

MICROFILM REEL NO: 005048 FRAME NO: 0242  
 NUMBER OF CLAIMS: 14

AB A compound of formula (I) or a pharmaceutically acceptable salt thereof:

# D R A W I N G

wherein: R1 is hydrogen, C1-6 alkyl, phenyl or phenyl C1-4 alkyl wherein the phenyl moiety is optionally substituted by one or more C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, hydroxy, C2-7 alkanoyl, halo, trifluoromethyl, nitro, amino optionally substituted by one or two C1-6 alkyl groups or by C2-7 alkanoyl, cyano, carbamoyl or carboxy groups; R2, R3 and R4 are independently selected from hydrogen, C1-6 alkyl, C1-6 alkoxy, C1-6 alkoxycarbonyl, C1-6 alkylthio, hydroxy, C2-7 alkanoyl, chloro, fluoro, trifluoromethyl, nitro, amino optionally substituted by one or two C1-6 alkyl groups or by C2-7 alkanoyl, cyano, carbamoyl and carboxy, and phenyl, phenyl C1-4 alkyl or phenyl C1-4 alkoxy in which any phenyl moiety is optionally substituted by any of these groups; R5 and R6 are independently selected from hydrogen, C1-6 alkyl, C3-7 cycloalkyl, C3-7 cycloalkyl-C1-4 alkyl, C2-6 alkenyl, C1-7 alkanoyl, C1-6 alkylsulphonyl, di-(C1-6 alkyl)amino C1-6 alkyl, 3-oxobutyl, 3hydroxybutyl, phenyl, phenyl C1-4 alkyl, benzoyl, phenyl C2-7 alkanoyl or benzenesulphonyl any of which phenyl moieties are optionally substituted by one or two halogen, C1-6 alkyl, C1-6 alkoxy, CF3, amino or carboxy, or R5 and R6 together are C2-6 polymethylene optionally interrupted by oxygen or NR9 wherein R9 is hydrogen or C1-6 alkyl optionally substituted by hydroxy; R7 is hydrogen, C1-6 alkyl, C3-6 cycloalkyl, C3-6 cycloalkyl-C1-4 alkyl, C2-6 alkenyl or C2-6 alkynyl; and -CO2R8 is a pharmaceutically acceptable ester group, processes for its preparation and its use for the treatment or prophylaxis of anxiety or depression.

CLMN 14

TI H-PYRIDO(2,3-B)INDOLE-3-CARBOXYLIC ACID ESTER

COMPOUNDS HAVING USEFUL PHARMACEUTICAL ACTIVITY; TREATMENT OF PROPHYLAXIS OF ANXIETY OR DEPRESSION

ACLM 8. 4-Amino-2-methyl-9H-pyrido(2,3-b)indole

-3-carboxylic acid, methyl ester, 4-amino-2,9-dimethyl-9H-pyrido

(2,3-b)indole-3-carboxylic acid, methyl ester,

4-amino-2-methyl-9H-pyrido(2,3-b)indole-3-carboxylic

acid, ethyl ester, 4-amino-6-chloro-2,9-dimethyl-9H-pyrido

(2,3-b)indole-3-carboxylic acid, methyl ester,

4-amino-9-methyl-2-phenyl-9H-pyrido(2,3-b)indole

-3-carboxylic acid, methyl ester, 4-n-butylamino-2,9-dimethyl-9H-

N-((5-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((6-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((7-Hydroxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalaninamide; N-((2,7-Dimethyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-tyrosine methyl ester; N-((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-3-methyl-L-valine methyl ester; N2-((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-N,N-dimethyl-L-phenylalaninamide; (1S)-N-(1-(Hydroxymethyl)-2-phenylethyl)-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indole-3-**carboxamide**; N-((2-Methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; 7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-N-(1,3,3-trimethylbicyclo(2.2.1)heptan-2-yl)-1H-indole-3-**carboxamide**; (alpha S)-alpha-(((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)amino)-2-thiophenepropanoic acid methyl ester; N-((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-6-aza-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((7-Methoxy-1-(2-(4-morpholinyl)ethyl)-1H-indazol-3-yl)carbonyl)-L-phenylalanine methyl ester; 7-Methoxy-1-(2-(4-morpholinyl)ethyl)-N-(1,3,3-trimethylbicyclo(2.2.1)heptan-2-yl)-1H-indazol-3-**carboxamide**; N-((7-Methoxy-1-(2-(4-morpholinyl)ethyl)-1H-indazol-3-yl)carbonyl)-R-amphetamine; (alpha S)-alpha-(((7-Methoxy-2-methyl-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)amino)-2-thiazolepropanoic acid methyl ester; 7-Methoxy-2-methyl-N-((1S)-1-(3-methyl)-tetrazolyl)-2-phenylethyl)-1-(2-(4-morpholinyl)ethyl)-1H-indole-3-**carboxamide**; 7-Methoxy-2-methyl-N-((1S)-1-(2-methyl)-tetrazolyl)-2-phenylethyl)-1-(2-(4-morpholinyl)ethyl)-1H-indole-3-**carboxamide**; N-((7-Methoxy-1-(2-(4-morpholinyl)ethyl)-1H-indol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((7-Methoxy-1-(2-(4-morpholinyl)ethyl)-1H-indazol-3-yl)carbonyl)-1-naphthyl amide; 7-Methoxy-1-(2-(4-morpholinyl)ethyl)-N-(1,3,3-trimethylbicyclo(2.2.1)heptan-2-yl)-1H-indole-3-**carboxamide**; 2-Methyl-1-(2-(4-morpholinyl)ethyl)-N-(1,3,3-trimethylbicyclo(2.2.1)heptan-2-yl)-1H-pyrrole-3-**carboxamide**; 2,5-Dimethyl-N-((1R)-1-methyl-2-phenylethyl)-1-(2-(4-morpholinyl)ethyl)-1H-pyrrole-3-**carboxamide**; N-((2,5-Dimethyl-1-(2-(4-morpholinyl)ethyl)-1H-pyrrol-3-yl)carbonyl)-L-phenylalanine methyl ester; N-((2-Methyl-1-(2-(4-morpholinyl)ethyl)-1H-pyrrol-3-yl)carbonyl)-L-phenylalanine methyl ester; 2-Methyl-N-((1S)-1-(3-methyl-1,2,4-oxadiazol-5-yl)-2-phenylethyl)-1-(2-(4-morpholinyl)ethyl)-1H-pyrrole-3-**carboxamide**; N-((1-(2-(4-Morpholinyl)ethyl)-1H-imidazol-4-yl)carbonyl)-L-phenylalanine methyl ester; N-((1-(2-Phenoxyethyl)-1H-imidazol-4-yl)carbonyl)-L-phenylalanine methyl ester; and N-((1-Pentyl-1H-imidazol-4-yl)carbonyl)-L-phenylalanine methyl ester; and (ii) a pharmaceutically-acceptable salt or hydrate thereof.

=> d his

(FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005)

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

```
L1      4000 S B(W) CARBOLIN?
L2      29 S 3-HYDROXAMIC(3A)ACID
L3      0 S L1 AND L2
L4      2431 S PYRIDO(4A)INDOL?
L5      0 S L2 AND L4
L6      17060 S CARBOXAMIDE
```

L7 108 S L1 AND L6  
 L8 1536 S RAUWOLFIA  
 L9 117 S NORHARMANE  
 L10 7516 S L1 OR L4 OR L8 OR L9  
 L11 23223 S "HYDROXAMIC ACID" OR CARBOXAMIDE  
 L12 148 S L10 AND L11  
 L13 143 S "CARBOXYLIC ACID" (4A) HYDROXY (3A) AMIDE  
 L14 23352 S L11 OR L13  
 L15 149 S L10 AND L14  
 L16 1 S L15 NOT L12

INDEX 'CAOLD, CAPLUS, CASREACT, CROPU, DGENE, DPCI, ENCOMPPAT, EPFULL,  
 FRANCEPAT, FRFULL, FSTA, IFIPAT, IMSPATENTS, INPADOC, JAPIO, KOREAPAT,  
 LITALERT, NTIS, PAPERCHEM2, PATDD, PATDPA, PATDPAFULL, PCTFULL, PCTGEN,  
 PIRA, PROUSDDR, PS, RAPRA, RDISCLOSURE, ...' ENTERED AT 17:00:01 ON 14  
 MAR 2005

SEA L15

149 FILE CAPLUS  
 20 FILE CASREACT  
 4 FILE DGENE  
 3 FILE DPCI  
 1 FILE ENCOMPPAT  
 216 FILE EPFULL  
 2 FILE FRANCEPAT  
 11 FILE FRFULL  
 68 FILE IFIPAT  
 24 FILE INPADOC  
 1 FILE JAPIO  
 1 FILE KOREAPAT  
 2 FILE NTIS  
 7 FILE PATDPAFULL  
 251 FILE PCTFULL  
 60 FILE PROUSDDR  
 5 FILE SYNTHLINE  
 839 FILE USPATFULL  
 108 FILE USPAT2  
 16 FILE WPIDS  
 16 FILE WPINDEX

L17 QUE L15

FILE 'IFIPAT' ENTERED AT 17:04:06 ON 14 MAR 2005

L18 68 S L15

=> fil beilstein

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
257.96	372.39

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-15.33

CA SUBSCRIBER PRICE

FILE 'BEILSTEIN' ENTERED AT 17:13:49 ON 14 MAR 2005

COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften  
 licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002

FILE LAST UPDATED ON February 14, 2005

FILE COVERS 1771 TO 2004.

\*\*\* FILE CONTAINS 9,133,317 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

**NEW**

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> s L15

360373 B  
    (BETA)  
    9855 CARBOLIN?  
    9559 B(W)CARBOLIN?  
    50432 PYRIDO  
    210416 INDOL?  
    9421 PYRIDO(4A)INDOL?  
    362 RAUWOLFIA  
    2 NORHARMANE  
    159 "HYDROXAMIC"  
2956171 "ACID"  
    560 "ACIDS"  
2956481 "ACID"  
    ("ACID" OR "ACIDS")  
    148 "HYDROXAMIC ACID"  
        ("HYDROXAMIC" (W) "ACID")  
    11207 CARBOXAMIDE  
    591511 "CARBOXYLIC"  
2956171 "ACID"  
    560 "ACIDS"  
2956481 "ACID"  
    ("ACID" OR "ACIDS")  
    591312 "CARBOXYLIC ACID"  
        ("CARBOXYLIC" (W) "ACID")  
    955798 HYDROXY  
    142153 AMIDE  
    48 AMIDES  
    142197 AMIDE  
        (AMIDE OR AMIDES)  
    3219 "CARBOXYLIC ACID" (4A)HYDROXY (3A)AMIDE  
L19      118 L10 AND L14

=> d L19 ibib abs 100-118

'IBIB' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'  
'ABS' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'

The following are valid formats:

QRD ----- Query Related Data (IDE plus HIT)  
IDE ----- Identification of Substance, plus Structure  
ALL ----- All Display fields (Lengthy displaye)  
CHE ----- Chemical Data  
PHY ----- Physical Data  
HIT ----- All fields containing hit terms  
Hit terms will be highlighted in all IDE fields in the BEILSTEIN file  
A maximum of 20 values are displayed in each single property field.  
Use DISPLAY F<prop> for FULL format, e.g. FBP instead of BP.  
For more information about display formats, and how to display  
individual selected properties, enter 'HELP FORMAT' at an arrow  
prompt, e.g. => HELP FORMAT.  
ENTER DISPLAY FORMAT (QRD):end

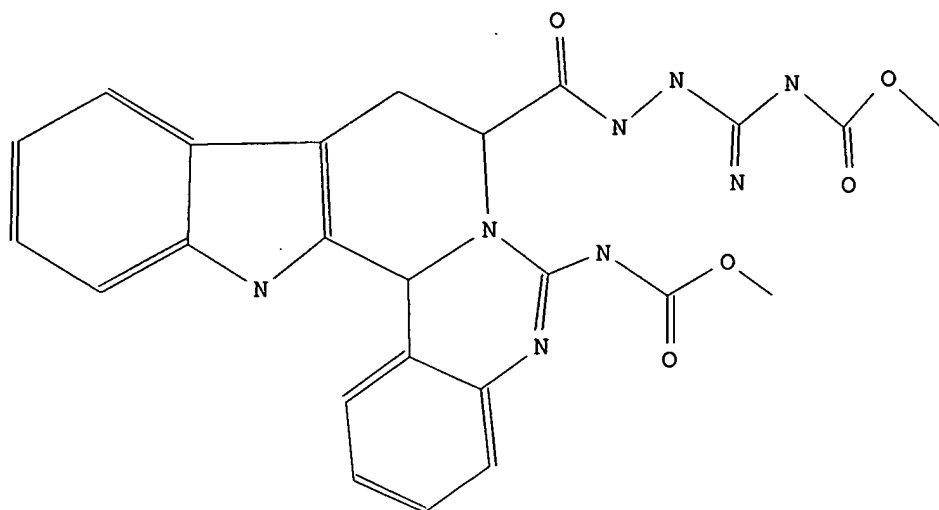
=> d L19 ti,au,so hit 100-118  
'AU' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'  
'SO' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'

The following are valid formats:

QRD ----- Query Related Data (IDE plus HIT)  
IDE ----- Identification of Substance, plus Structure  
ALL ----- All Display fields (Lengthy displaye)  
CHE ----- Chemical Data  
PHY ----- Physical Data  
HIT ----- All fields containing hit terms  
Hit terms will be highlighted in all IDE fields in the BEILSTEIN file  
A maximum of 20 values are displayed in each single property field.  
Use DISPLAY F<prop> for FULL format, e.g. FBP instead of BP.  
For more information about display formats, and how to display  
individual selected properties, enter 'HELP FORMAT' at an arrow  
prompt, e.g. => HELP FORMAT.  
ENTER DISPLAY FORMAT (QRD):qrd

L19 ANSWER 100 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4577464
Beilstein Pref. RN (BPR):	107292-70-6
CAS Reg. No. (RN):	107292-70-6
Chemical Name (CN):	<b>1,3,4,9-Tetrahydro-1-(2-hydroxy-2-methylcyclohexyl)-N-2-propenyl-2H-pyrido&lt;3,4-b&gt;indole-2-carboxamide</b>
Autonom Name (AUN):	<b>1-(2-hydroxy-2-methyl-cyclohexyl)-1,3,4,9-tetrahydro-<math>\beta</math>-carboline-2-carboxylic acid allylamide</b>
Molec. Formula (MF):	C22 H29 N3 O2
Molecular Weight (MW):	367.49
Lawson Number (LN):	28394, 2947, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	4126534
Tautomer ID (TAUTID):	4409340
Beilstein Citation (BSO):	6-23
Entry Date (DED):	1991/12/02
Update Date (DUPD):	1993/03/20



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d L19 qrd 1-79

L19 ANSWER 1 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN):

Chemical Name (CN):

Autonom Name (AUN):

Molec. Formula (MF):

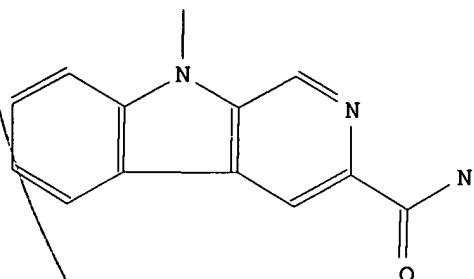
9627510

**N-methyl-β-carboline-3-carboxamide**, FG 7142

**9-methyl-9H-β-carboline-3-carboxylic acid amide**

C13 H11 N3 O

Molecular Weight (MW): 225.25  
 Lawson Number (LN): 29236, 2817  
 Compound Type (CTYPE): heterocyclic  
 Constitution ID (CONSID): 8114843  
 Tautomer ID (TAUTID): 9026611  
 Entry Date (DED): 2004/07/21  
 Update Date (DUPD): 2004/07/21



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	2
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
CPD	Crystal Property Description	1
MP	Melting Point	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	3
PHARM	Pharmacological Data	1

L19 ANSWER 2 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9588969  
 Chemical Name (CN): (+/-) trans-1-(4-methoxyphenyl)-N-(phenylmethyl)-2,3,4,9-tetrahydro-1H-pyrido<3,4-b>indole-3-carboxamide  
 Autonom Name (AUN): 1-(4-methoxy-phenyl)-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid benzylamide  
 Molec. Formula (MF): C26 H25 N3 O2  
 Molecular Weight (MW): 411.50  
 Lawson Number (LN): 29323, 14140, 289  
 File Segment (FS): racemate, Stereo compound  
 Compound Type (CTYPE): heterocyclic  
 Constitution ID (CONSID): 8085068  
 Tautomer ID (TAUTID): 8998276  
 Entry Date (DED): 2004/04/23  
 Update Date (DUPD): 2004/04/23

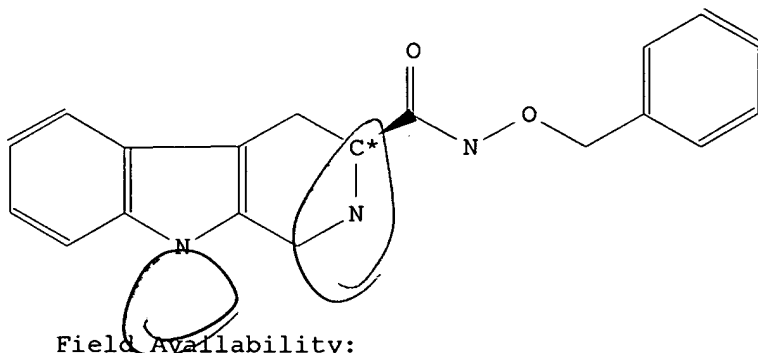


This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L19 ANSWER 7 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

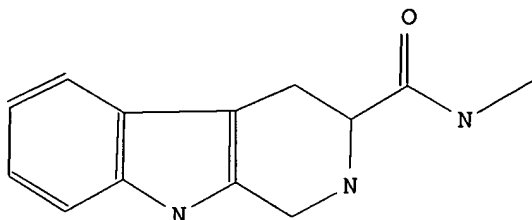
Beilstein Records (BRN): 9076718  
Chemical Name (CN): (3R)-N-benzyloxy-1,3,4,9-tetrahydro-  
β-carboline-3-carboxamide  
Autonom Name (AUN): 2,3,4,9-tetrahydro-1H-β-  
carboline-3-carboxylic acid  
benzyloxy-amide  
Molec. Formula (MF): C19 H19 N3 O2  
Molecular Weight (MW): 321.38  
Lawson Number (LN): 29228, 5228  
File Segment (FS): Stereo compound  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 7670629  
Tautomer ID (TAUTID): 8530244  
Entry Date (DED): 2002/07/19  
Update Date (DUPD): 2002/07/19



Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Constitution ID (CONSID): 4009099  
 Tautomer ID (TAUTID): 6213514  
 Beilstein Citation (BSO): 6-25  
 Entry Date (DED): 1994/04/18  
 Update Date (DUPD): 1994/04/18



Fragment Notes:  
 Stereo Descriptor: D

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

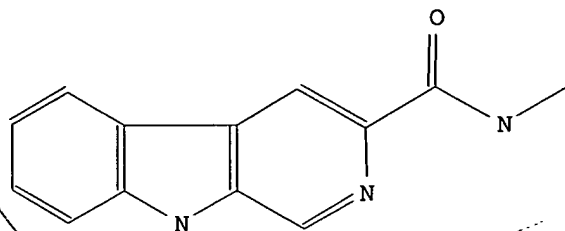
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L19 ANSWER 73 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6569956  
 Chemical Name (CN): **N-methyl  $\beta$ -carboline-3-carboxamide**  
 Autonom Name (AUN): **9H- $\beta$ -carboline-3-carboxylic acid methylamide**  
 Molec. Formula (MF): C13 H11 N3 O  
 Molecular Weight (MW): 225.25  
 Lawson Number (LN): 29236, 2817  
 Compound Type (CTYPE): heterocyclic  
 Constitution ID (CONSID): 5657806

Tautomer ID (TAUTID): 6209964  
 Beilstein Citation (BSO): 6-25  
 Entry Date (DED): 1994/04/18  
 Update Date (DUPD): 2004/04/23



Field Availability:

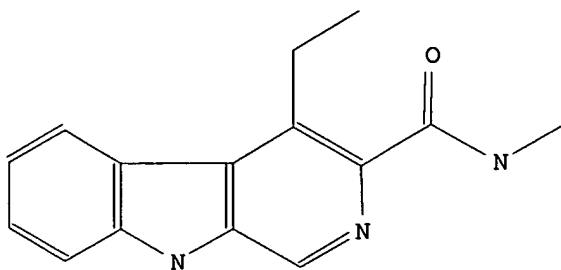
Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
COEV	Concentration in Environment	2
MP	Melting Point	1
MS	Mass Spectrum	1
PHARM	Pharmacological Data	16
UVS	UV and Visible Spectrum	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	5
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	4

L19 ANSWER 74 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6526501  
 Chemical Name (CN): **L-N-n-octyl-1,2,3,4-tetrahydro-β-carboline-3-carboxamide**  
 Autonom Name (AUN): **2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid octylamide**  
 Molec. Formula (MF): C20 H29 N3 O  
 Molecular Weight (MW): 327.47  
 Lawson Number (LN): 29228, 2872  
 File Segment (FS): Stereo compound  
 Compound Type (CTYPE): heterocyclic



Field Availability:

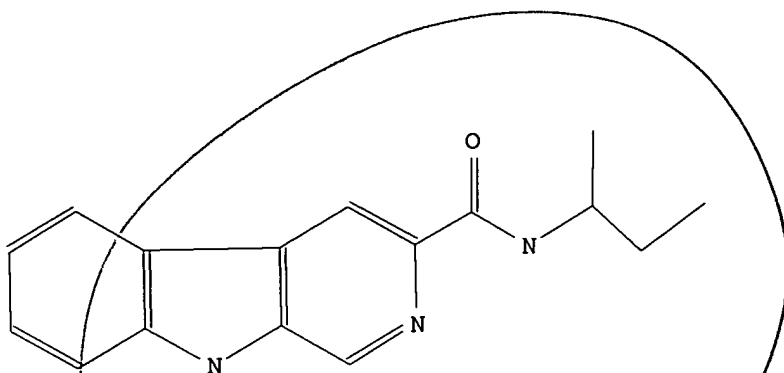
Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L19 ANSWER 78 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6515214  
 Chemical Name (CN): **N-sec-butyl- $\beta$ -carboline-3-carboxamide**  
 Autonom Name (AUN): **9H- $\beta$ -carboline-3-carboxylic acid**  
**sec-butyl-amide**  
 Molec. Formula (MF): C16 H17 N3 O  
 Molecular Weight (MW): 267.33  
 Lawson Number (LN): 29236, 2845  
 Compound Type (CTYPE): heterocyclic  
 Constitution ID (CONSID): 5664652  
 Tautomer ID (TAUTID): 6219571  
 Beilstein Citation (BSO): 6-25  
 Entry Date (DED): 1994/04/18  
 Update Date (DUPD): 1994/04/18



Field Availability:

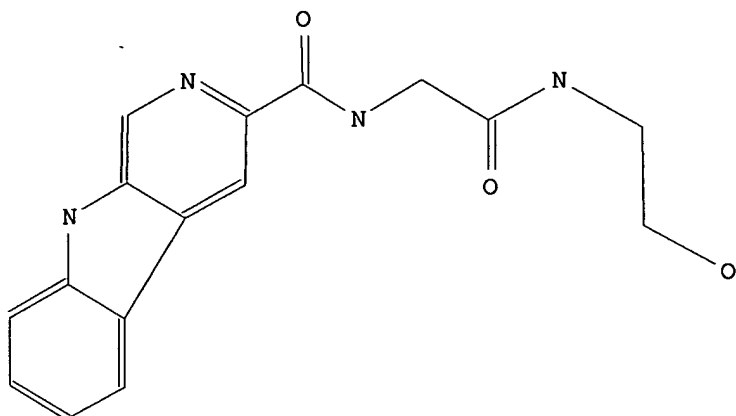
Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

L19 ANSWER 79 OF 118 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6234187  
 Chemical Name (CN): **9H-β-carboline-3-carboxylic acid  
 <(2-hydroxy-ethylcarbamoyl)-methyl>-amide**  
 Autonom Name (AUN): **9H-β-carboline-3-carboxylic acid  
 <(2-hydroxy-ethylcarbamoyl)-methyl>-amide**  
 Molec. Formula (MF): C16 H16 N4 O3  
 Molecular Weight (MW): 312.33  
 Lawson Number (LN): 29236, 3379, 3122  
 Compound Type (CTYPE): heterocyclic  
 Constitution ID (CONSID): 5445089  
 Tautomer ID (TAUTID): 5951410  
 Beilstein Citation (BSO): 6-25  
 Entry Date (DED): 1993/10/20  
 Update Date (DUPD): 1993/10/20



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> fil caold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
1200.90	1573.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-15.33

FILE 'CAOLD' ENTERED AT 17:23:00 ON 14 MAR 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s L15

```
31490 BETA
      5 BETAS
31495 B
      (BETA OR BETAS)
      235 CARBOLIN?
      105 B(W) CARBOLIN?
      145 PYRIDO
4038 INDOL?
      13 PYRIDO(4A) INDOL?
      594 RAUWOLFIA
      3 RAUWOLFIA
      597 RAUWOLFIA
      (RAUWOLFIA OR RAUWOLFIA)
      2 NORHARMANE
      294 "HYDROXAMIC"
145227 "ACID"
68234 "ACIDS"
203842 "ACID"
      ("ACID" OR "ACIDS")
      285 "HYDROXAMIC ACID"
      ("HYDROXAMIC" (W) "ACID")
      132 CARBOXAMIDE
      120 CARBOXAMIDES
      251 CARBOXAMIDE
      (CARBOXAMIDE OR CARBOXAMIDES)
      6430 "CARBOXYLIC"
145227 "ACID"
68234 "ACIDS"
203842 "ACID"
      ("ACID" OR "ACIDS")
      5819 "CARBOXYLIC ACID"
      ("CARBOXYLIC" (W) "ACID")
      8841 HYDROXY
      1810 AMIDE
      3891 AMIDES
      5642 AMIDE
      (AMIDE OR AMIDES)
      28 "CARBOXYLIC ACID" (4A) HYDROXY (3A) AMIDE
L20      0 L10 AND L14
```

=> d his

(FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005)

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

```
L1      4000 S B(W) CARBOLIN?
L2      29 S 3-HYDROXAMIC (3A) ACID
L3      0 S L1 AND L2
```

L4 2431 S PYRIDO(4A)INDOL?  
 L5 0 S L2 AND L4  
 L6 17060 S CARBOXAMIDE  
 L7 108 S L1 AND L6  
 L8 1536 S RAUWOLFIA  
 L9 117 S NORHARMANE  
 L10 7516 S L1 OR L4 OR L8 OR L9  
 L11 23223 S "HYDROXAMIC ACID" OR CARBOXAMIDE  
 L12 148 S L10 AND L11  
 L13 143 S "CARBOXYLIC ACID"(4A)HYDROXY(3A)AMIDE  
 L14 23352 S L11 OR L13  
 L15 149 S L10 AND L14  
 L16 1 S L15 NOT L12

INDEX 'CAOLD, CAPLUS, CASREACT, CROPU, DGENE, DPCI, ENCOMPPAT, EPFULL,  
 FRANCEPAT, FRFULL, FSTA, IFIPAT, IMSPATENTS, INPADOC, JAPIO, KOREAPAT,  
 LITALERT, NTIS, PAPERCHEM2, PATDD, PATDPA, PATDPAFULL, PCTFULL, PCTGEN,  
 PIRA, PROUSDDR, PS, RAPRA, RDISCLOSURE, ...' ENTERED AT 17:00:01 ON 14  
 MAR 2005

SEA L15

149 FILE CAPLUS  
 20 FILE CASREACT  
 4 FILE DGENE  
 3 FILE DPCI  
 1 FILE ENCOMPPAT  
 216 FILE EPFULL  
 2 FILE FRANCEPAT  
 11 FILE FRFULL  
 68 FILE IFIPAT  
 24 FILE INPADOC  
 1 FILE JAPIO  
 1 FILE KOREAPAT  
 2 FILE NTIS  
 7 FILE PATDPAFULL  
 251 FILE PCTFULL  
 60 FILE PROUSDDR  
 5 FILE SYNTHLINE  
 839 FILE USPATFULL  
 108 FILE USPAT2  
 16 FILE WPIDS  
 16 FILE WPINDEX

L17 QUE L15

FILE 'IFIPAT' ENTERED AT 17:04:06 ON 14 MAR 2005

L18 68 S L15

FILE 'BEILSTEIN' ENTERED AT 17:13:49 ON 14 MAR 2005

L19 118 S L15

FILE 'CAOLD' ENTERED AT 17:23:00 ON 14 MAR 2005

L20 0 S L15

=> fil casreact

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
23.83	1597.12

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-15.33

CA SUBSCRIBER PRICE



FILE 'CASREACT' ENTERED AT 17:23:48 ON 14 MAR 2005  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 13 Mar 2005 VOL 142 ISS 11

```
*****
*
*      CASREACT now has more than 8 million reactions      *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L15

```
72060 BETA
  2 BETAS
72060 B
      (BETA OR BETAS)
  876 CARBOLIN?
  670 B(W)CARBOLIN?
 2571 PYRIDO
14476 INDOL?
  431 PYRIDO(4A)INDOL?
   30 RAUWOLFIA
   6 NORHARMANE
   1 NORHARMANES
   7 NORHARMANE
      (NORHARMANE OR NORHARMANES)
  762 "HYDROXAMIC"
168074 "ACID"
 53611 "ACIDS"
178282 "ACID"
      ("ACID" OR "ACIDS")
  738 "HYDROXAMIC ACID"
      ("HYDROXAMIC" (W) "ACID")
 2506 CARBOXAMIDE
 1233 CARBOXAMIDES
 3208 CARBOXAMIDE
      (CARBOXAMIDE OR CARBOXAMIDES)
24558 "CARBOXYLIC"
   6 "CARBOXYLICS"
24559 "CARBOXYLIC"
      ("CARBOXYLIC" OR "CARBOXYLICS")
168074 "ACID"
 53611 "ACIDS"
178282 "ACID"
      ("ACID" OR "ACIDS")
 23349 "CARBOXYLIC ACID"
      ("CARBOXYLIC" (W) "ACID")
 48529 HYDROXY
 14760 AMIDE
 10936 AMIDES
```

## 20403 AMIDE

(AMIDE OR AMIDES)

21 "CARBOXYLIC ACID" (4A) HYDROXY (3A) AMIDE

L21 20 L10 AND L14

=&gt; d L21 1-20 ibib abs

L21 ANSWER 1 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 140:111299 CASREACT

TITLE: Unexpected ipso-substitutions at the  $\beta$  -  
**carboline** nucleus

AUTHOR(S): Kast, Oliver; Bracher, Franz

CORPORATE SOURCE: Zentrum fuer Pharmaforschung, Department Pharmazie,  
Ludwig-Maximilians-Universitaet, Munich, GermanySOURCE: Synthetic Communications (2003), 33(22), 3843-3850  
CODEN: SYNCAV; ISSN: 0039-7911

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Minisci-type radical carbamoylation of 1-bromo- $\beta$  -  
**carboline** (I) gives the 3-substituted product in low yield,  
whereas 1-acetyl- $\beta$  -**carboline** (II) reacts under  
ipso-substitution of the acetyl group. Cyanations of the N-oxides of I  
and II occur under clean ipso-substitution of the groups in 1-position.  
1-Me derivs. show no tendency to react under ipso-substitution.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:381394 CASREACT

TITLE: Synthesis and characterization of the aqueous solution  
chemistry of the food-derived carcinogen model  
N-acetoxy-N-(1-methyl-5H-**pyrido**[4,5-b]  
**indol**-3-yl)acetamide and its N-pivaloyloxy  
analogueAUTHOR(S): Rajagopal, Sridharan; Brooks, Michael E.; Nguyen,  
Thach-Mien; Novak, MichaelCORPORATE SOURCE: Hughes Laboratory, Department of Chemistry and  
Biochemistry, Miami University, Oxford, OH, 45056, USA

SOURCE: Tetrahedron (2003), 59(40), 8003-8010

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of N-acetyl-N-(acetyloxy)-1-methyl-5H-**pyrido**  
[4,3-b]**indol**-3-amine (I) and N-acetyl-N-(2,2-dimethyl-1-  
oxopropoxy)-1-methyl-5H-**pyrido**[4,3-b]**indol**-3-amine  
(II) were reported. In aqueous solution at neutral pH, I primarily undergoes

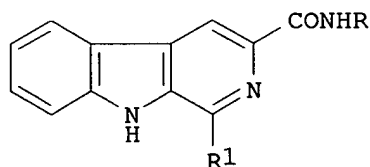
C-O  
bond cleavage to yield the **hydroxamic acid**, 8, but  
under the same conditions the sterically hindered II decomps.  
predominately by N-O bond cleavage with a pH independent rate constant that  
is 7.5-fold smaller than that for I. In the pH range 0.5-7.0 three  
different processes for the decomposition of II were detected by kinetics.  
Only the process that dominates at neutral pH generates a nitrenium  
species that can be trapped by N-3.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

hydroxyl, dihydroxy, carboxyl,  $-C(O)NRaRb$ ,  $-NRaRb$ ,  $-NRaC(O)NRaRb$ ,  $-NRaC(O)ORa$ ,  $-OC(O)NRaRb$ , or  $-NHC(O)Ra$ . R2 is H or a (un)substituted alkyl (substituent = hydroxyl, dihydroxyl, carboxyl,  $-C(O)NRaRb$ ,  $-NRaRb$ ,  $-NRaC(O)NRaRb$ ,  $-NRaC(O)ORa$ ,  $-OC(O)NRaRb$ , or  $-NHC(O)Ra$ ), or R1, R2 and N together form a substituted piperazine, substituted azetidine, or a pyrrolidine ring substituted with  $-(CH_2)_2OH$  or  $-CH_2C(O)OH$ . R3 is a (un)substituted Ph or a 5-6 membered heteroaryl ring, wherein the substituent is halogen, hydroxyl, cyano, (C1-C15)alkyl, (C1-C15)alkoxyl or  $-NRaRb$ ; R4 is H or (un)substituted (C1-C15)alkyl; R5 is  $-(CH_2)_mOR_6$ ,  $-CHNOR_7$ ,  $-C(O)NR_8R_9$ ,  $-(CH_2)_mC(O)OR_{10}$ ,  $-(CH_2)_kC(O)NR_{11}R_{12}$ ; addnl. details are given in the claims. Radioligand binding assays yielded selectivities for the A2b receptor relative to the A1, A2a and A3 receptors for 9 examples of I, e.g. 26 times for II. About 26 example preps. of I and intermediates and characterization data for hundreds of I and intermediates are included. For example, III can be prepared by reacting 4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine with  $PhSO_2Cl$  and a reducing agent in the presence of solvent to produce 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine, which was reacted with  $CO_2$  in the presence of LDA and a solvent to produce lithium 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylate, which was reacted with  $AcNHCH_2CH_2NH_2$  in the presence of solvent to give 4-(2-acetylaminoethylamino)-7-benzenesulfonyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, which was deprotected with a hydroxide base and subsequently condensed with amines.

L21 ANSWER 6 OF 20 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 136:340858 CASREACT  
 TITLE: Synthesis of  $\beta$ -**carboline**-3-**carboxamides** and their interaction with DNA  
 AUTHOR(S): Lin, Wei; Xiao, Sulong; Yang, Ming  
 CORPORATE SOURCE: National Laboratory of Natural and Biomimetic Drugs, Peking University, Beijing, 100083, Peop. Rep. China  
 SOURCE: Beijing Daxue Xuebao, Yixueban (2001), 33(3), 277-279  
 CODEN: BDXYAH  
 PUBLISHER: Beijing Daxue  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 GI

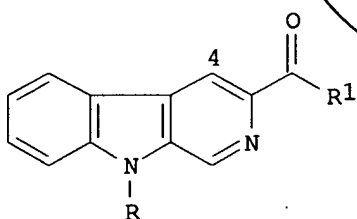


I

AB Title compds. I (R1 = H or Me; R = 2-aminoethyl, 6-aminoethyl, 2-diethylaminoethyl, or 3-dimethylaminopropyl) were synthesized from tryptophan via esterification with methanol, cyclization with formaldehyde in the presence of 28%  $NH_4OH$ , oxidation with  $Pb(OAc)_4$ , and substitution with  $RNH_2$ . The interaction between the synthetic compds. with DNA was studied. There was intercalation reaction of the synthetic compds. with DNA. The  $IC_{50}$  of the synthetic compds. to HL-60, KB, HeLa, and BGC cells was presented. The  $\delta T_m$  of the synthetic compds. to CT-DNA, thermodyn. parameters at  $25^\circ$  for the synthetic compds. binding on DNA, and intrinsic binding consts. and number of binding sites for the synthetic compds. with CT-DNA were presented.

-3-(N-phenyl) **carboxamide** with methyllithium, iodine and Me iodide. I in the presence of catalytic palladium acetate and tri-o-tolylphosphine in acetonitrile and triethylamine reacted with a variety of unsatd. substrates (styrenes, acrylate, tributyl(vinyl)tin, trimethylsilylacetylene) to give the corresponding C-4 coupled adducts.  
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

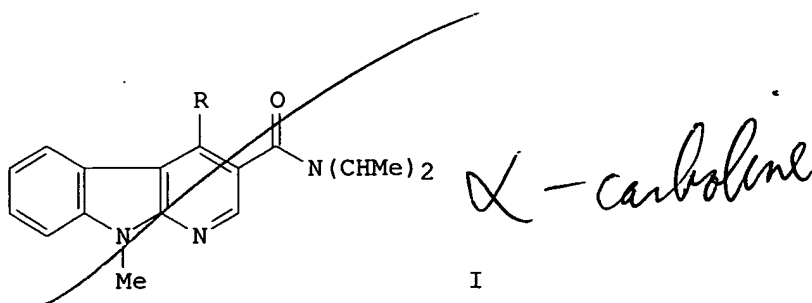
L21 ANSWER 9 OF 20 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 124:117133 CASREACT  
TITLE: Regioselective metalation of 9-methoxymethyl-  
**beta.-carboline-3-**  
**carboxamides** with amidomagnesium chlorides  
AUTHOR(S): Schlecker, Wolfgang; Huth, Andreas; Ottow, Eckhard;  
Mulzer, Johann  
CORPORATE SOURCE: Schering AG Berlin, Berlin, D-13353, Germany  
SOURCE: Synthesis (1995), (10), 1225-7  
CODEN: SYNTBF; ISSN: 0039-7881  
PUBLISHER: Thieme  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The N-protected  $\beta$  -**carbolines** I (R = CH<sub>2</sub>OMe; R<sub>1</sub> = NHCMe<sub>3</sub>, NHMe) underwent exclusive metalation at C(4) with R<sub>2</sub>MgCl (R<sub>2</sub> = 2,2,6,6-tetramethylpiperidino) and/or Et<sub>2</sub>NMgCl, whereas the unprotected **beta.-carboline** I (R = H; R<sub>1</sub> = NHMe) was inert under these conditions. The C(4) metalated species reacted with electrophiles to give 3,4-disubstituted  $\beta$  -**carbolines**, which are interesting precursors to physiol. active compds.

L21 ANSWER 10 OF 20 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 121:205309 CASREACT  
TITLE: Study of the lithiation of 3-substituted  
 $\alpha$ -carbolines. A new route to 3,4-disubstituted  
derivatives  
AUTHOR(S): Papamicael, Cyril; Dupas, Georges; Bourguignon, Jean;  
Queguiner, Guy  
CORPORATE SOURCE: Inst. Natl. Sci. Appliquees Rouen, CNRS,  
Mont-Saint-Aignan, 76131, Fr.  
SOURCE: Tetrahedron Letters (1994), 35(24), 4099-102  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

*alpha* <sup>no</sup> -carboline



AB The preparation of new 3-substituted  $\alpha$ -carbolines (1H- **pyrido** [2,3-b]**indole** derivs.) was described and these products were subjected to ortho-lithiation expts. 3-Pivalamido and 3-carboxamido derivs. are cleanly lithiated at 4-position. The results are correlated with MNDO calcs. Various 3,4-disubstituted  $\alpha$ -carbolines are obtained in excellent yields. Thus, 9-methyl-N,N-diisopropyl-1H-**pyrido**[2,3-b]**indole**-3-**carboxamide** I (R = H) was treated with lithium 2,2,6,6-tetramethylpiperidine and quenched with Et formate to give I (R = CO<sub>2</sub>Et) in 72% yield.

L21 ANSWER 11 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 113:184209 CASREACT

TITLE: Potent anticonflict activity and lessening of memory impairment with a series of novel [1]benzothieno[2,3-c]pyridines and 1,2,3,4-tetrahydro[1]benzothieno[2,3-c]pyridines

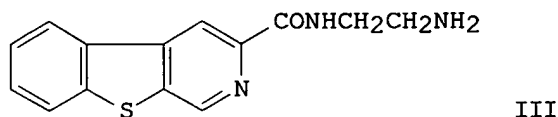
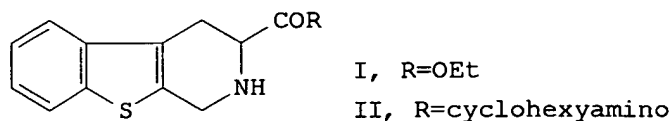
AUTHOR(S): Kawakubo, Hiromu; Okazaki, Katuya; Nagatani, Tadasi; Takao, Katuyuki; Hasimoto, Shinichi; Sugihara, Taisuke  
CORPORATE SOURCE: Inst. Life Sci., Asahi Chem. Ind. Co., Ltd., Nobeoka, 882, Japan

SOURCE: Journal of Medicinal Chemistry (1990), 33(11), 3110-16  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB [1]Benzothieno[2,3-c]pyridines and 1,2,3,4-tetrahydro[1]benzothieno[2,3-c]pyridines were synthesized. The compds. are bioisosteres of **beta.-carbolines** and 1,2,3,4-tetrahydro-**beta.-carbolines** where the indole N is replaced by S. Their pharmacol. activity was evaluated in a water lick conflict test in rats and a passive avoidance test in mice. In the 1,2,3,4-tetrahydro[1]benzothieno[2,3-c]pyridine series, the presence of Et ester (I) or cyclohexylcarboxamide (II) groups at C-3 conferred good anticonflict activity and lessening of memory impairment, while N-acylation of I abolished activity. In the [1]benzothieno[2,3-c]pyridine series, the aminoethyl **carboxamide** (III) group at C-3 also

conferred activity, but other amides studied were not active. The most potent compds. (I, II, and III) were administered orally and had potent anticonflict and scopolamine-amnesia reversal activity. These compds. did not bind to the benzodiazepine receptor in spite of having structures similar to those of  $\beta$ -**carboline**s. III bound strongly to 5-HT<sub>1A</sub> receptors and thus is expected to be a novel anxiolytic.

L21 ANSWER 12 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 111:97121 CASREACT

TITLE: Synthesis and benzodiazepine receptor affinities of rigid analogs of 3-carboxy- $\beta$ -**carboline**s: demonstration that the

benzodiazepine receptor recognizes preferentially the s-cis conformation of the 3-carboxy group

AUTHOR(S): Dorey, Gilbert; Poissonnet, Guillaume; Potier, Marie Claude; De Carvalho, Lia Prado; Venault, Patrice; Chapouthier, Georges; Rossier, Jean; Potier, Pierre; Dodd, Robert H.

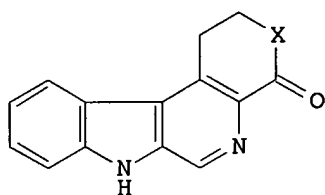
CORPORATE SOURCE: Inst. Chim. Subst. Nat., Gif-sur-Yvette, F 91198, Fr.  
SOURCE: Journal of Medicinal Chemistry (1989), 32(8), 1799-804

CODEN: JMCMAR; ISSN: 0022-2623

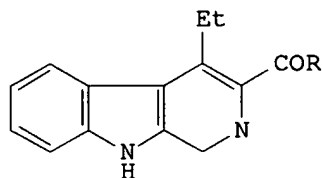
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



III

AB Indolopyrido-2-penten-5-olide I (X = O; II) and indolopyridopyridinone I (X = NH), rigid analogs of Me 4-ethyl- $\beta$ -**carboline** -3-carboxylate III (R = OMe; IV) and N-methyl-4-ethyl- $\beta$ -**carboline**-3-**carboxamide** III (R = NHMe; V), resp., were synthesized and their in vitro binding affinities to the central type benzodiazepine receptors were compared. The IC<sub>50</sub> values of II and IV were approx. equivalent (42 and 27 nM, resp.). The amide derivative V, for which theor. energy calcns. indicate that the s-trans carbonyl conformation is the preferred one, displayed very low affinity (IC<sub>50</sub> > 104 nM). However, when the carbonyl group of V was forced to adopt the s-cis conformation as in lactam I (X = NH), binding to the benzodiazepine receptor was largely restored (IC<sub>50</sub> = 150 nM), indicating that the s-cis carboxy conformation at C-3 of  $\beta$ -**carboline**s is preferentially recognized by this receptor. In vivo, II showed neither convulsant, proconvulsant, nor anticonvulsant activity in mice. Moreover, II did not antagonize Me  $\beta$ -**carboline**-3-carboxylate induced convulsions in mice. This lack of activity of II was attributed to its inability to cross the blood-brain barrier since no significant displacement of [<sup>3</sup>H]Ro 15-1788 from mouse brain benzodiazepine receptors by II could be observed in vivo.

L21 ANSWER 13 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

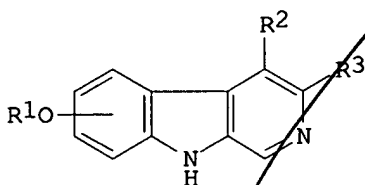
ACCESSION NUMBER: 109:128862 CASREACT

TITLE: Synthesis of substituted **pyrido**[3,4-b]

EP 237467 B1 19921028  
 R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE  
 HU 43605 A2 19871130 HU 1987-977 19870306  
 HU 196204 B 19881028  
 AT 81857 E 19921115 AT 1987-730022 19870306  
 CA 1315784 A1 19930406 CA 1987-531388 19870306  
 ES 2052598 T3 19940716 ES 1987-730022 19870306  
 AU 8769885 A1 19870910 AU 1987-69885 19870309  
 AU 593331 B2 19900208  
 JP 62270580 A2 19871124 JP 1987-52243 19870309  
 JP 07116184 B4 19951213  
 US 4877792 A 19891031 US 1987-23752 19870309  
 US 4960777 A 19901002 US 1989-409899 19890920  
 DE 1986-3608089 19860308  
 EP 1987-730022 19870306  
 US 1987-23752 19870309

PRIORITY APPLN. INFO.:

GI



*rw*

AB The title compds. [I; R1 = (substituted) heteroaryl; R2 = H, alkyl, alkoxyalkyl; R3 = carboxylate, **carboxamide**, carboxyalkyl, (substituted) oxadiazolyl] were prepared as central nervous system agents (no data). Me2NCH:C(CO2Et)N:CHNMe2 was stirred 10 min with HOAc and CF3CO2H. 4-(2-Pyrazinyloxy)indole was added and the mixture was stirred at room temperature for 24 h and at reflux for 2 h to give 56% I [R1O = 5-(2-pyrazinyloxy), R2 = H, R3 = CO2Et].

L21 ANSWER 15 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 107:96702 CASREACT

TITLE: Phenoxy- $\beta$ -**carboline**

INVENTOR(S): derivatives as central nervous system agents  
 Schmiechen, Ralph; Seidelmann, Dieter; Huth, Andreas;  
 Schneider, Herbert Hans; Stephens, David Norman;  
 Engelstoft, Mogens; Hansen, John Bondo; Petersen,  
 Erling

PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 13 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

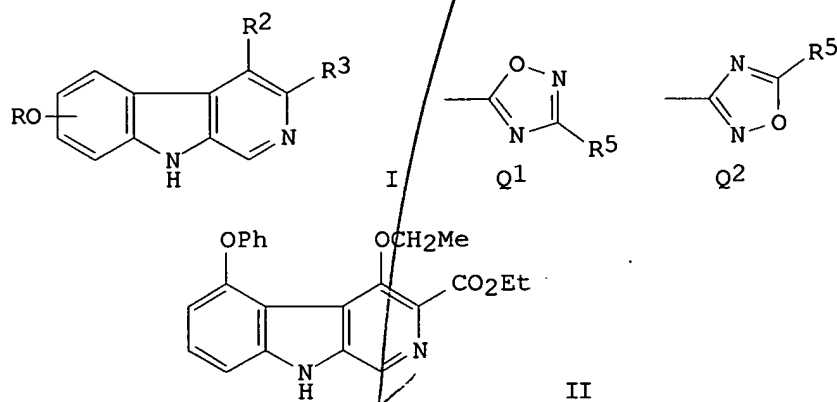
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3540654	A1	19870514	DE 1985-3540654	19851113
EP 234173	A2	19870902	EP 1986-730188	19861111
EP 234173	A3	19880706		
EP 234173	B1	19930616		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 90678	E	19930715	AT 1986-730188	19861111
ES 2058064	T3	19941101	ES 1986-730188	19861111

NO 8604517	A	19870514
NO 163736	B	19900402
NO 163736	C	19900711
HU 43067	A2	19870928
HU 198046	B	19890728
DD 254201	A5	19880217
CA 1269377	A1	19900522
IL 80618	A1	19900917
DK 8605438	A	19870514
DK 169702	B1	19950116
FI 8604619	A	19870514
FI 84067	B	19910628
FI 84067	C	19911010
AU 8665170	A1	19870521
AU 602497	B2	19901018
ZA 8608631	A	19870624
JP 62167780	A2	19870724
JP 06099431	B4	19941207
US 4945090	A	19900731
FI 85480	B	19920115
FI 85480	C	19920427

NO 1986-4517	19861112
HU 1986-4678	19861112
DD 1986-296211	19861112
CA 1986-522771	19861112
IL 1986-80618	19861112
DK 1986-5438	19861113
FI 1986-4619	19861113
AU 1986-65170	19861113
ZA 1986-8631	19861113
JP 1986-268799	19861113
US 1986-929861	19861113
FI 1989-5790	19891204
DE 1985-3540654	19851113
EP 1986-730188	19861111
FI 1986-4619	19861113

PRIORITY APPLN. INFO.:

GI



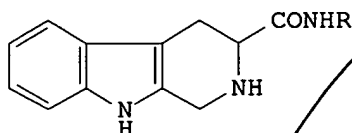
AB The title compds. (I; R = C<sub>6</sub>H<sub>4</sub>R<sub>1</sub>; R<sub>1</sub> = H, halo, alkyl, alkoxy, acyloxy, Ph, alkylendioxy, CF<sub>3</sub>, cyano, NO<sub>2</sub>, N<sub>3</sub>, alkoxycarbonyl, sulfonyl, sulfonamido; R<sub>2</sub> = H, alkyl, alkoxyalkyl; R<sub>3</sub> = Q<sub>1</sub>, Q<sub>2</sub>, CO<sub>2</sub>R<sub>4</sub>, **carboxamide**; R<sub>4</sub> = alkyl; R<sub>5</sub> = H, alkyl, cycloalkyl) were prepared as CNS (central nervous system) agents. Et 5-hydroxy-4-(methoxymethyl)-**beta**-**carboline**-3-carboxylate was heated with 4-FC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub> in DMF at 100° to give the 5-(4-nitrophenyl) derivative, which was reduced to the corresponding amine using H/Pd/C in MeOH/THF. The amine was diazotized with HBF<sub>4</sub>/NaNO<sub>2</sub> and the diazo compound treated in situ with hypophosphorus acid to give phenoxy-**beta**-**carboline** derivative II. II had an ED<sub>50</sub> of 0.4 mg/mL i.p. for displacement of 3H-flunitrazepam from diazepam receptors in mouse brains.

L21 ANSWER 16 OF 20 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 100:209657 CASREACT  
 TITLE: Some 3-**carboxamides** of **beta**-

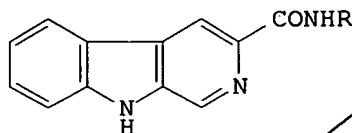


**carboline and tetrahydro- $\beta$ -carboline**

AUTHOR(S): Coutts, Ronald T.; Micetich, Ronald G.; Baker, Glen B.; Benderly, Abraham; Dewhurst, Tim; Hall, Tse Wei; Locock, Anthony R.; Pyrozko, Jerry  
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Alberta, Edmonton, AB, T6G 2N8, Can.  
SOURCE: Heterocycles (1984), 22(1), 131-42  
CODEN: HTCYAM; ISSN: 0385-5414  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I



II

AB L- And D-tetrahydro- $\beta$ -**carboline**-3-**carboxamides** I (R = H, C1-12 alkyl, cycloalkyl) were made by the interaction of RNH<sub>2</sub> with Me tetrahydro- $\beta$ -**carboline**-3-carboxylate. The  $\beta$ -**carboline**-3-**carboxamides** II were prepared from Me  $\beta$ -**carboline**-3-carboxylate or by aromatization of I. The diastereomers I (R = CHMeEt) were separated by chromatog.

L21 ANSWER 17 OF 20 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 71:112783 CASREACT  
TITLE: Reductive decyanization of  $\alpha$ -amino nitriles with sodium borohydride. Synthetic approach to isoquinoline and indole alkaloids  
AUTHOR(S): Yamada, Shunichi; Akimoto, Hiroshi  
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan  
SOURCE: Tetrahedron Letters (1969), (36), 3105-8  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Various types of  $\alpha$ -amino nitriles, PhCH<sub>2</sub>CH(CN)NHAc (I), PhCH<sub>2</sub>CH(CN)NMe<sub>2</sub> (II), and III (R = CN), readily prepared by dehydration of  $\alpha$ -amino acid amide derivs. with POCl<sub>3</sub>, were decyanized by NaBH<sub>4</sub> reduction I heated with NaBH<sub>4</sub> 24 hrs. in diglyme at 100° yielded 88% PhCH<sub>2</sub>CH<sub>2</sub>NHAc; II similarly heated with NaBH<sub>4</sub> 20 hrs. at 35° in EtOH gave 100% PhCH<sub>2</sub>CH<sub>2</sub>NMe, also obtained in 87% yield by reductive decyanization 24 hrs. at 60° in C<sub>5</sub>H<sub>5</sub>N. Decyanization of III under optimal conditions (20 hrs. at 35° in EtOH) yielded III (R = H). L-Tryptophan converted by treatment with AcH and esterification with alc. HCl into the optically pure ester IV (R = CO<sub>2</sub>Et, R<sub>1</sub> = H) (IVa), m. 116°, [ $\alpha$ ]<sub>24D</sub> - 106° (c 0.4, alc.) and treated with NH<sub>3</sub>-MeOH gave the corresponding **carboxamide** IV (R = CO-NH<sub>2</sub>, R<sub>1</sub> = H) (V), m. 114°, [ $\alpha$ ]<sub>25D</sub> - 149° (c 0.4, EtOH). V benzoylated with PhCH<sub>2</sub>Br and NaHCO<sub>3</sub> in alc. and dehydrated with POCl<sub>3</sub> gave the amino nitrile IV (R = CN, R<sub>1</sub> = CH<sub>2</sub>Ph) (VI), m. 160-1°, [ $\alpha$ ]<sub>23D</sub> - 12.6° (c 1.6, C<sub>5</sub>H<sub>5</sub>N). VI decyanized with NaBH<sub>4</sub> in EtOH-C<sub>5</sub>H<sub>5</sub>N and debenzylated by catalytic hydrogenation gave optically pure 1-methyl-1,2,3,4-tetrahydro- $\beta$ -**carboline** (VII), m. 177°, [ $\alpha$ ]<sub>25D</sub> - 52° (c 2.0, alc.). The asym. center of (-)-VII was shown to have (S)-configuration. The optically pure initial

corresponding benzyl chloride. VII were prepared mainly from RCl or RBr with 2 mol ArNH<sub>2</sub> without a solvent above 100°, but some were obtained by reduction of the corresponding Schiff bases. IV (R = Z = H) (18.6 g.) converted to its Na derivative by boiling 1-2 h. with 4.5 g. PhMe-moistened NaNH<sub>2</sub> in 150 cc. absolute PhMe or xylene, with ClCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub> added, and the crude base distilled, gave 70% IV (R = Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, Z = H), b<sub>2.5</sub> 200-5°; maleate, C<sub>24</sub>H<sub>31</sub>N<sub>3</sub>O<sub>8</sub>, m. 164-5° (from MeOH-Et<sub>2</sub>O); 73% IV (R = Et<sub>2</sub>NCO, Z = H) (VIIa) was similarly obtained using Et<sub>2</sub>NCOCl and precipitating from solution in Me<sub>2</sub>CO or MeOH as the naphthalene-1,5-disulfonate, m. 265-7° (from HOAc-Me<sub>2</sub>CO) [VIIa.HCl, m. 202-3° (from alc.-Et<sub>2</sub>O)]. Similar reactions using PhCH<sub>2</sub>Cl succeeded poorly or not at all, apparently as the result of extensive quaternization at the 3-position. IVa (27.6 g.) in 250 cc. Me<sub>2</sub>CO, refluxed 24 h. with 18 g. PhCH<sub>2</sub>Cl, gave 81% 3-methyl-3,9-dibenzyl-1,2,3,4-tetrahydro-γ-carbolinium chloride, m. 211-12° (from alc.-Et<sub>2</sub>O); at room temperature IVa treated with 14 g. Me<sub>2</sub>SO<sub>4</sub> and the product precipitated by 250 cc. Et<sub>2</sub>O gave 90% 3,3-dimethyl-9-benzyl-1,2,3,4-tetrahydro-γ-carbolinium methosulfate, m. 217-18° (from alc.-Et<sub>2</sub>O). The Na derivative of 1-methyl-4-imino-3-cyanopiperidine (from 69 g. MeN(CH<sub>2</sub>CH<sub>2</sub>CN)<sub>2</sub> in PhMe, filtered off under N, and washed with PhMe) was added carefully under CO<sub>2</sub> to 250 g. concentrated H<sub>2</sub>SO<sub>4</sub> in 1 l. H<sub>2</sub>O, the aqueous layer separated, 35 g. PhNHNH<sub>2</sub>, and 100 g. 20% H<sub>2</sub>SO<sub>4</sub> added, the mixture refluxed 6-8 h., and made alkaline giving Cl<sub>3</sub>H<sub>16</sub>N<sub>4</sub>, m. 123° (from C<sub>6</sub>H<sub>6</sub>), which may be the phenylhydrazone of 1-methyl-3-cyano-4-piperidone or VIII. α-(p-Methoxybenzylamino)pyridine (IX), m. 128°, was converted to the nitroso derivative, m. 56-7° (from ligroine), and reduced with Zn dust; some IX was recovered from the concentrated Et<sub>2</sub>O exts. by precipitation with ligroine and crude N,N-(p-methoxybenzyl)-α-pyridylhydrazine (X) was obtained by evaporation of the filtrate. X (20 g.) in 120 cc. alc. was treated in the cold with HCl, 14 g. V.HCl added, the mixture heated slightly on the water bath, then 2-3 h. at 70-80°, and Me<sub>2</sub>CO added to precipitate 5 g. V α-pyridylhydrazone-HCl, m. 224-5° (from MeOH-Me<sub>2</sub>CO); this was converted through the free base to the dimaleate, m. 142-3° (from alc. Et<sub>2</sub>O), and the dipicrate, m. 202-3° (from 90% HOAc-Et<sub>2</sub>O).

=> d his

(FILE 'HOME' ENTERED AT 16:47:52 ON 14 MAR 2005)

FILE 'CAPLUS' ENTERED AT 16:48:12 ON 14 MAR 2005

```

L1      4000 S B(W)CARBOLIN?
L2      29 S 3-HYDROXAMIC(3A)ACID
L3      0 S L1 AND L2
L4      2431 S PYRIDO(4A)INDOL?
L5      0 S L2 AND L4
L6      17060 S CARBOXAMIDE
L7      108 S L1 AND L6
L8      1536 S RAUWOLFIA
L9      117 S NORHARMANE
L10     7516 S L1 OR L4 OR L8 OR L9
L11     23223 S "HYDROXAMIC ACID" OR CARBOXAMIDE
L12     148 S L10 AND L11
L13     143 S "CARBOXYLIC ACID" (4A)HYDROXY(3A)AMIDE
L14     23352 S L11 OR L13
L15     149 S L10 AND L14
L16     1 S L15 NOT L12

```

INDEX 'CAOLD, CAPLUS, CASREACT, CROPU, DGENE, DPCI, ENCOMPPAT, EPFULL, FRANCEPAT, FRFULL, FSTA, IFIPAT, IMSPATENTS, INPADOC, JAPIO, KOREAPAT,

LITALERT, NTIS, PAPERCHEM2, PATDD, PATDPA, PATDPAFULL, PCTFULL, PCTGEN,  
PIRA, PROUSDDR, PS, RAPRA, RDISCLOSURE, ...' ENTERED AT 17:00:01 ON 14  
MAR 2005

SEA L15  
-----

149 FILE CAPLUS  
20 FILE CASREACT  
4 FILE DGENE  
3 FILE DPCI  
1 FILE ENCOMPPAT  
216 FILE EPFULL  
2 FILE FRANCEPAT  
11 FILE FRFULL  
68 FILE IFIPAT  
24 FILE INPADOC  
1 FILE JAPIO  
1 FILE KOREAPAT  
2 FILE NTIS  
7 FILE PATDPAFULL  
251 FILE PCTFULL  
60 FILE PROUSDDR  
5 FILE SYNTHLINE  
839 FILE USPATFULL  
108 FILE USPAT2  
16 FILE WPIDS  
16 FILE WPINDEX

L17 QUE L15  
-----

L18 FILE 'IFIPAT' ENTERED AT 17:04:06 ON 14 MAR 2005  
68 S L15

L19 FILE 'BEILSTEIN' ENTERED AT 17:13:49 ON 14 MAR 2005  
118 S L15

L20 FILE 'CAOLD' ENTERED AT 17:23:00 ON 14 MAR 2005  
0 S L15

L21 FILE 'CASREACT' ENTERED AT 17:23:48 ON 14 MAR 2005  
20 S L15

=> fil dissabs

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	74.89	1672.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-13.60	-28.93

FILE 'DISSABS' ENTERED AT 17:25:39 ON 14 MAR 2005

COPYRIGHT (C) 2005 ProQuest Information and Learning Company; All Rights Reserved.

FILE COVERS 1861 TO 25 FEB 2005 (20050225/ED)

Only fair use as provided by the United States copyright law is permitted. PROQUEST INFORMATION AND LEARNING COMPANY MAKES NO WARRANTY REGARDING THE ACCURACY, COMPLETENESS OR TIMELINESS OF THE LICENSED MATERIALS OR ANY WARRANTY, EXPRESS OR IMPLIED, INCLUDING ANY WARRANTY OF MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE, AND SHALL NOT BE LIABLE FOR DAMAGES OF ANY KIND OR LOST PROFITS OR OTHER CLAIMS RELATED TO THE LICENSED MATERIALS OR THEIR USE.

=> s L15

38836 BETA  
242 BETAS  
38947 B  
    (BETA OR BETAS)  
133 CARBOLIN?  
117 B(W) CARBOLIN?  
98 PYRIDO  
2300 INDOL?  
18 PYRIDO(4A) INDOL?  
25 RAUWOLFIA  
3 NORHARMANE  
175 "HYDROXAMIC"  
64081 "ACID"  
23265 "ACIDS"  
75304 "ACID"  
    ("ACID" OR "ACIDS")  
169 "HYDROXAMIC ACID"  
    ("HYDROXAMIC" (W) "ACID")  
191 CARBOXAMIDE  
57 CARBOXAMIDES  
236 CARBOXAMIDE  
    (CARBOXAMIDE OR CARBOXAMIDES)  
2663 "CARBOXYLIC"  
1 "CARBOXYLICS"  
2664 "CARBOXYLIC"  
    ("CARBOXYLIC" OR "CARBOXYLICS")  
64081 "ACID"  
23265 "ACIDS"  
75304 "ACID"  
    ("ACID" OR "ACIDS")  
2363 "CARBOXYLIC ACID"  
    ("CARBOXYLIC" (W) "ACID")  
4856 HYDROXY  
2775 AMIDE  
1077 AMIDES  
3504 AMIDE  
    (AMIDE OR AMIDES)  
1 "CARBOXYLIC ACID" (4A) HYDROXY (3A) AMIDE  
L22 3 L10 AND L14

=> d L22 ibib abs

L22 ANSWER 1 OF 3 DISSABS COPYRIGHT (C) 2005 ProQuest Information and Learning Company; All Rights Reserved on STN  
ACCESSION NUMBER: 2003:13549 DISSABS Order Number: AAI3057227  
TITLE: Synthesis and reactivity of food derived promutagens and procarcinogens IQx and Trp-P-2  
AUTHOR: Brooks, Michael Edward [Ph.D.]; Novak, Michael [adviser]  
CORPORATE SOURCE: Miami University (0126)  
SOURCE: Dissertation Abstracts International, (2002) Vol. 63, No. 6B, p. 2842. Order No.: AAI3057227. 98 pages.  
ISBN: 0-493-72421-4.  
DOCUMENT TYPE: Dissertation  
FILE SEGMENT: DAI  
LANGUAGE: English  
AB N-acetyl-N-acetoxy-2-amino-3-methylaminoimidazo[4,5-f]quinoxaline, N-Ac-N-OAc-IQx, 2, was synthesized as a model derivative of the food derived mutagen and carcinogen IQx, 1. The decomposition kinetics showed pH dependence that is consistent with the uncatalyzed decomposition of the neutral form of 2. The products of the decomposition in phosphate and acetate buffers were identified. Addition of nucleophiles N 3- and dG at

neutral pH did not affect the rate of decomposition of 2. This is also consistent with the formation of a nitrenium ion intermediate as the rate determining step during the decomposition of 2. The  $k_{az}/k_s$  and  $k_dG/K_s$  selectivity ratios were determined to be  $(5.2 \pm 0.5) + 104 M^{-1}$  and  $(9.1 \pm 2.1) + 102 M^{-1}$ , respectively. The structure of the product at neutral pH and also in the presence of the added nucleophiles is consistent with the formation of a nitrenium ion intermediate during the decomposition of 2. In the presence of dG, both the C-8 and N-2 adducts were isolated. The major adduct formed in the presence of dG was the C-8 adduct.

*Use* 3-(N-Acetoxy-N-acetyl)-amino-1-methyl-5H-pyrido[4,3-b]indole, N-OAc-N-Ac-Trp-P-2, 4, was synthesized as a model derivative of the food derived mutagen and carcinogen Trp-P-2, 3. The kinetics of the decomposition of 4 show that there are two consecutive processes at most pH values. One of the processes corresponds to the disappearance of 4 according to HPLC studies. The compound 4 showed pH-dependent hydrolysis kinetics that is consistent with the uncatalyzed decomposition of the neutral form and the acid catalyzed decomposition of the protonated form. The pKa of the compound was determined by the kinetic method to be  $3.84 \pm 0.08$ . The ester 4 undergoes acid catalyzed ester hydrolysis to generate the corresponding **hydroxamic acid** at pH < 1.6.

=> d L22 ibib abs 2-3

L22 ANSWER 2 OF 3 DISSABS COPYRIGHT (C) 2005 ProQuest Information and Learning Company; All Rights Reserved on STN  
ACCESSION NUMBER: 81:21303 DISSABS Order Number: AAR8117660  
TITLE: A STUDY OF THE REISSERT COMPOUND CHEMISTRY OF SOME DIAZAHETEROCYCLIC SYSTEMS  
AUTHOR: VEERARAGHAVAN, SESHADRI [PH.D.]  
CORPORATE SOURCE: UNIVERSITY OF MISSOURI - KANSAS CITY (0134)  
SOURCE: Dissertation Abstracts International, (1981) Vol. 42, No. 3B, p. 1026. Order No.: AAR8117660. 135 pages.  
DOCUMENT TYPE: Dissertation  
FILE SEGMENT: DAI  
LANGUAGE: English  
ENTRY DATE: Entered STN: 19921118  
Last Updated on STN: 19921118

AB The Reissert compound chemistry of several diazaheterocyclic bases such as the (alpha)-, (beta)- and (gamma)-carbolines, the pyrido(4,3-b)carbazoles, pyrrolo(1,2-a)quinoxaline, pyrrolo(2,3-b)pyridine, pyridazine, pyrimidine, pyrazine, quinine and pyrido(2,3-b)pyrazine (a triaza system) was investigated. (alpha)-, (beta)- and (delta)-Carbolines failed to form Reissert compounds under a wide variety of conditions. Pyrrolo(2,3-b)pyridine also failed to afford a Reissert compound. 3,4-Dihydro-(**beta**)-**carboline**, however, yielded the corresponding Reissert compound either by the phase transfer catalyst method or by the trimethylsilyl cyanide method. The 3,4-dihydro-(**beta**)-**carboline** Reissert compound underwent alkylation with alkyl halides in the presence of a base, but the subsequent alkaline hydrolysis of the alkylated Reissert compounds did not lead to the anticipated 1-alkyl-3,4-dihydro-(**beta**)-**carbolines** but to the formation of 1-alkyl-1,2,3,4-tetrahydro-(**beta**)-**carboline**-1-carboxamides. Oxidation of the 3,4-dihydro-(**beta**)-**carboline** Reissert compound with 2,3-dichloro-5,6-dicyanobenzoquinone (DDQ) yielded 1-cyano-(**beta**)-**carboline**. Treatment of 1-cyano-(**beta**)-**carboline** with ethanolic potassium hydroxide resulted in the alkaloid, 1-carbamoyl-(**beta**)-**carboline**. Several analogs of the 3,4-dihydro-(**beta**)-**carboline** Reissert compound were also prepared and

A quantitative study of DMT metabolism was conducted in whole brain homogenate obtained from rodents which had not been pretreated with iproniazid. In this study  $6.0 \times 10^{-8}$  M 5-((<sup>3</sup>H)-DMT was metabolized to DMT-NO, NMT, indole-3-acetic acid (IAA) and 2-methyl-1,2,3,4-tetrahydro-(**beta**)-**carboline** (2-MTHBC). The major metabolite over a two hour incubation period was IAA, with formation of the other metabolites having peaked at or before 30 minutes. Incubation of  $2.0 \times 10^{-5}$  M 5-((<sup>3</sup>H)-DMT gave DMT-NO as the major metabolite after 30 minutes. The formation of NMT peaked at one hour and IAA production appeared to be inhibited during the entire two-hour incubation period. The formation of 2-MTHBC, however, steadily increased over this time period. When 5-((<sup>3</sup>H)-DMT-NO was used as a substrate DMT and NMT were formed. Anaerobic incubation enhanced DMT and NMT formation and led to the production of 2-MTHBC as a metabolite. When whole brain homogenate from rodents pretreated with the MAOI iproniazid was used as the enzyme source, IAA formation was found to be inhibited by 83%. However, this MAOI also inhibited NMT and DMT-NO formation by 90% and no 2-MTHBC was observed to be formed.

In brain microsomes obtained from non-iproniazid treated rodents 5-((<sup>3</sup>H)-DMT was converted to DMT-NO, IAA and NMT. The metabolism of DMT was dependent on NADPH, nicotinamide (NA), Mg(<sup>2+</sup>) and O<sub>2</sub>. DMT was not metabolized under anaerobic conditions or in the presence of an N-oxidase inhibitor, 1-(1-naphthyl)-2-thiourea. Incubation of 5-((<sup>3</sup>H)-DMT-NO gave DMT and IAA as metabolites. Anaerobic incubation of DMT-NO gave 2-MTHBC as the major metabolite and enhanced formation of NMT, DMT and IAA.

The formation of DMT-NO is postulated as a major factor in the overall metabolism of DMT and a cyclic pathway for the in vitro and possible in vivo metabolism and synthesis of DMT is proposed.

Following the identification of 2-MTHBC as an in vitro metabolite of DMT, experiments were conducted to determine if this compound was normally formed in vivo. Using rodent whole brain extracts, analyses were conducted by GC/MS with known standards. Using the method of selected ion monitoring the compounds 2-MTHBC and its demethylated analog, 1,2,3,4-tetrahydro-(**beta**)-**carboline** (THBC), were identified as normal constituents of rat brain. Possible mechanisms for the formation of these compounds from DMT and the other metabolites of DMT, i.e., NMT, DMT-NO and HCHO, are presented.

The tetrahydro-(**beta**)-**carbolines** are postulated to be putative neuroregulatory agents and/or hormone-like compounds regulating MAO activity and biogenic amine uptake. The possibility that these compounds are involved in certain psychopathological conditions is proposed. Preliminary data indicate that THBC is present in blood serum from some schizophrenic subjects.

Several N(,1)-alkyl-1,2,5,6-tetrahydropyridine-3-(N,N-diethyl) **carboxamides** (THPC), analogs of the D ring of LSD, were prepared and tested for their ability to block the behavioral effects of DMT in two rodent behavior paradigms. In both a food and a water reinforcement schedule paradigm 30 minutes pretreatment of rats with IP injected N(,1)-allyl- or N(,1)-propyl-THPC (10.0 and 20.0 mg/kg) significantly inhibited the effects of DMT (5.0 mg/kg IP). If DMT is involved in schizophrenia certain of these compounds may be clinically useful.

=> fil wpids

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
------------------	---------------

FULL ESTIMATED COST

7.72	1679.73
------	---------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
------------------	---------------

CA SUBSCRIBER PRICE

0.00	-28.93
------	--------

FILE 'WPIDS' ENTERED AT 17:27:00 ON 14 MAR 2005

COPYRIGHT (C) 2005 THE THOMSON CORPORATION

FILE LAST UPDATED: 11 MAR 2005 <20050311/UP>  
MOST RECENT DERWENT UPDATE: 200517 <200517/DW>  
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,  
PLEASE VISIT:  
[http://www.stn-international.de/training\\_center/patents/stn\\_guide.pdf](http://www.stn-international.de/training_center/patents/stn_guide.pdf) <<<

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE  
<http://thomsonderwent.com/coverage/latestupdates/> <<<

>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER  
GUIDES, PLEASE VISIT:  
<http://thomsonderwent.com/support/userguides/> <<<

>>> NEW! FAST-ALERTING ACCESS TO NEWLY-PUBLISHED PATENT  
DOCUMENTATION NOW AVAILABLE IN DERWENT WORLD PATENTS INDEX  
FIRST VIEW - FILE WPIFV.  
FOR FURTHER DETAILS: <http://www.thomsonderwent.com/dwpifv> <<<

>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501.  
PLEASE CHECK:  
<http://thomsonderwent.com/support/dwpioref/reftools/classification/code-revision/>  
FOR DETAILS. <<<

=> s L15

114510 BETA  
41 BETAS  
114522 B  
(BETA OR BETAS)  
454 CARBOLIN?  
341 B(W) CARBOLIN?  
2288 PYRIDO  
17562 INDOL?  
347 PYRIDO(4A) INDOL?  
114 RAUWOLFIA  
3 NORHARMANE  
1 NORHARMANES  
4 NORHARMANE  
(NORHARMANE OR NORHARMANES)  
1343 "HYDROXAMIC"  
887548 "ACID"  
164392 "ACIDS"  
925128 "ACID"  
("ACID" OR "ACIDS")  
1271 "HYDROXAMIC ACID"  
("HYDROXAMIC" (W) "ACID")  
5465 CARBOXAMIDE  
950 CARBOXAMIDES  
5962 CARBOXAMIDE  
(CARBOXAMIDE OR CARBOXAMIDES)  
123629 "CARBOXYLIC"  
8 "CARBOXYLICS"  
123632 "CARBOXYLIC"  
("CARBOXYLIC" OR "CARBOXYLICS")  
887548 "ACID"  
164392 "ACIDS"  
925128 "ACID"  
("ACID" OR "ACIDS")  
112205 "CARBOXYLIC ACID"  
("CARBOXYLIC" (W) "ACID")

127150 HYDROXY  
 2 HYDROXIES  
 127152 HYDROXY  
 (HYDROXY OR HYDROXIES)  
 57707 AMIDE  
 14220 AMIDES  
 67501 AMIDE  
 (AMIDE OR AMIDES)  
 208 "CARBOXYLIC ACID"(4A)HYDROXY(3A)AMIDE  
 L23 16 L10 AND L14

=> d L23 ibib abs 1-16

L23 ANSWER 1 OF 16 WPIDS COPYRIGHT 2005 THE THOMSON CORP on STN  
 ACCESSION NUMBER: 2005-081417 [09] WPIDS  
 DOC. NO. CPI: C2005-028171  
 TITLE: New tricyclic heterocyclic compounds, useful for  
 preventing/treating mitochondrial benzodiazepine receptor  
 accompanied disease such as stress-induced-central  
 nervous-, respiratory- and digestive system-disorders.  
 DERWENT CLASS: B02  
 INVENTOR(S): KATO, M; KATSUMATA, S; MANAKO, J; MATSUSHITA, T; OHMOTO,  
 K  
 PATENT ASSIGNEE(S): (ONOE) ONO PHARM CO LTD  
 COUNTRY COUNT: 108  
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2004113300	A1	20041229	(200509)*	JA	177
RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NA NL OA PL PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW W: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ OM PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW					

# APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004113300	A1	WO 2004-JP9071	20040622

PRIORITY APPLN. INFO: JP 2003-178436 20030623

AN 2005-081417 [09] WPIDS

AB WO2004113300 A UPAB: 20050207

NOVELTY - Tricyclic heterocyclic compounds (I) are new.

DETAILED DESCRIPTION - Tricyclic heterocyclic compounds of formula  
 A-X-Y'-Z'-B' (I) and their salts, N-oxides, solvates and prodrugs are new.

A = optionally substituted cyclic group;

X-Y'-Z' = bond or spacer; and

B' = optionally substituted hydrocarbon or cyclic group.

INDEPENDENT CLAIMS are also included for the following:

- (1) composition containing (I);
- (2) prophylactic or therapeutic agent of central nervous system-,  
 respiratory- and digestive system-disorders containing (I);
- (3) pharmaceutical containing (I), in combination with antianxiety-,  
 antidepressant-, anti-Parkinson-, antiepileptic-, antiasthmatic-, peptic  
 ulcer treating-, digestive tract function regulating-drug, antidiarrheal,  
 purgative, hypotensive, antiarrhythmic, cardiostonic, dysuria therapeutic  
 agent and integrated malfunction therapeutic agent; and



(4) use of (I) for manufacturing prophylactic/therapeutic agent of mitochondrial benzodiazepine receptor accompanied disease.

ACTIVITY - Tranquilizer; CNS-Gen.; Sedative; Antidepressant; Anticonvulsant; Respiratory-Gen.; Antiasthmatic; Gastrointestinal-Gen.; Antiinflammatory; Immunosuppressive; Neuroleptic; Nootropic; Antiparkinsonian; Neuroprotective; Antimigraine; Analgesic; Dermatological; Antiallergic; Antipruritic; Endocrine-Gen.

Mental stress was induced in Wister male rat and anti-stress effect of 2-acetyl-1-(3-fluorophenyl)-1,2,3,9-tetrahydro spiro(( **beta** )-**carboline**-4,1'-cyclopropane) (Ia) was evaluated according to method described in Brain research (BrainRes.), 641, 21-28 page, 1994. (Ia) was administered orally at a dose of 10 mg/kg. Bowel evacuation was counted after 1 hour. The result showed that (Ia) suppressed bowel evacuation number significantly, due to anti-stress effect of (Ia).

MECHANISM OF ACTION - Benzodiazepine-Agonist; Benzodiazepine-Antagonist.

Rat meninges sample extracted from whole brain of Wister male rat was used in receptor binding experiment and affinity of 2-acetyl-1-(3-fluorophenyl)-1,2,3,9-tetrahydro spiro(( **beta** )-**carboline**-4,1'-cyclopropane) (Ia) with respect to mitochondrial benzodiazepine receptor (MBR) was measured. (1-(2-chlorophenyl)-N-methyl-N-(1-methylpropyl)-3-isoquinoline **carboxamide**) described in European journal of pharmacology (Eur. J. pharmacol.), 119, 153-167 pages, 1985 ((3H)PK11195) was used as MBR selective ligand. Radioactivity was measured with liquid scintillation counter. Scatchard analysis was conducted using the obtained data and dissociation constant was obtained. Inhibition constant (Ki value) was calculated according to biochemical pharmacology (Biochem.Pharmacol.), 22, 3099-3108 page, 1973. The result showed that (Ia) had high affinity with respect to MBR with Ki value of 21 nM.

USE - For preventing or treating mitochondrial benzodiazepine receptor accompanied disease such as stress, and stress-induced-central nervous system disorders (such as uneasiness-associated disease, somniphathy, depression and/or epilepsy), stress-induced respiratory disorders (such as asthma) and stress-induced digestive system disorders (such as irritable bowel syndrome) (claimed). The uneasiness-associated disease is neurosis, psychosomatic disease, generalized/social anxiety disorder, panic-, attention deficit hyperactivity-, personality-, bipolar-disorders or autism. Other central nervous system disease are Parkinson's disease, schizophrenia, autonomic imbalance, Alzheimer's disease, emotional disorder, cognitive impairment, migraine, tension-headache and migrainous neuralgia. Several other central nervous system, respiratory and digestive system disorders are disclosed. (I) is also used for treating stress-induced dermal disease e.g. dermatitis, urticaria, eczema, skin pruritis, alopecia areata, etc.

ADVANTAGE - The compound (I) has high affinity to mitochondrial benzodiazepine receptor, produces very less toxicity and highly safe to use as pharmaceuticals.

Dwg.0/0

L23 ANSWER 2 OF 16 WPIDS COPYRIGHT 2005 THE THOMSON CORP on STN  
ACCESSION NUMBER: 2004-594157 [57] WPIDS  
DOC. NO. CPI: C2004-216170  
TITLE: New carbazole derivatives are HIV integrase inhibitors useful to treat diseases such as AIDS or AIDS related complex.  
DERWENT CLASS: B02  
INVENTOR(S): KUKI, A; LI, X; PLEWE, M B; WANG, H; ZHANG, J  
PATENT ASSIGNEE(S): (PFIZ) PFIZER INC  
COUNTRY COUNT: 108  
PATENT INFORMATION:

PATENT NO KIND DATE WEEK LA PG

WO 2004067531 A1 20040812 (200457)\* EN 57  
 RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE  
 LS LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW  
 W: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DE  
 DK DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG  
 KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ  
 OM PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG  
 US UZ VC VN YU ZA ZM ZW

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004067531	A1	WO 2004-IB259	20040123

*gum eff*

PRIORITY APPLN. INFO: US 2003-443223P 20030127

AN 2004-594157 [57] WPIDS

AB WO2004067531 A UPAB: 20040907

NOVELTY - Carbazole derivatives (I), (Ib) and their salts are new.

DETAILED DESCRIPTION - Carbazole derivatives of formula (I) or (Ib) and their salts are new.

R1-R6 = H, halo, 1-6C alkyl, alkoxy (1-6C alkyl), 2-6C alkenyl, 2-6C alkynyl, -ORc, -NO2 or -N(Rc)2;

Rc = H, 1-6C alkyl, 2-6C alkenyl or 2-6C alkynyl;

R7 = 1-6C alkyl, 2-6C alkenyl or 2-6C alkynyl (all optionally substituted by one or more substituents of halo, 1-6C alkyl, 2-6C alkenyl, 2-6C alkynyl, (hetero)cycloalkyl or (hetero)aryl (where aryl or (hetero)cycloalkyl are optionally substituted with one or more substituents of halo, 2-6C alkyl, 2-6C alkenyl, of 2-6C alkynyl)); and

R8, R9 = H, 1-6C alkyl, 2-6C alkenyl or 2-6C alkynyl (where alkyl, alkenyl or alkynyl are optionally substituted with one or more substituents of halo, (hetero)cycloalkyl or (hetero)aryl (where aryl or (hetero)cycloalkyl are optionally substituted with one or more substituents of halo, 1-6C alkyl, 2-6C alkenyl, or 2-6C alkynyl)).

A = (C(R10)(R11))n;

R10, R11 = H, halo, 1-6C alkyl, 2-6C alkenyl, 2-6C alkynyl, -ORc, or -N(Rc)2; and

n = 1-3.

ACTIVITY - Anti-HIV.

MECHANISM OF ACTION - HIV integrase inhibitor; HIV replication inhibitor. The ability of inhibit HIV integrase was assessed by integrase strand-transfer scintillation proximity assay. The results showed that median inhibitory concentration value of 9-(4-fluorobenzyl)-N-hydroxy-9H-beta-carboline-3-carboxamide was 0.234 mu M.

USE - (I) is useful in the treatment of diseases or conditions mediated by HIV integrase (claimed) such as AIDS or AIDS related complex (ARC).

Dwg. 0/0

L23 ANSWER 3 OF 16 WPIDS COPYRIGHT 2005 THE THOMSON CORP on STN

ACCESSION NUMBER: 2004-580628 [56] WPIDS

DOC. NO. CPI: C2004-211623

TITLE: Use of tryptanthrin compound and an antigen to enhance an immune response to treat e.g. cholera, typhoid, hepatitis B infection, influenza, rabies, measles, mumps, rubella, polio, yellow fever, tetanus and diphtheria.

DERWENT CLASS: B02 B04 B07

INVENTOR(S): VALIANTE, N M; VALIANTE, N

PATENT ASSIGNEE(S): (CHIR) CHIRON CORP

COUNTRY COUNT: 108

PATENT INFORMATION:

Considerable MAO inhibiting activity for treatment of mental depression in man and animals. Also strong anorexigenic and anti-inflammatory agent.

The known N'-dimethylindole-2-**carboxamide** is reduced to 1-methyl-2-methylaminomethylindole. Each mol. of this cpd. is reacted with 2-mol. equivalent of oxalyl chloride to give (I).

=> fil mrck

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	63.20	1742.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-28.93

FILE 'MRCK' ENTERED AT 17:27:52 ON 14 MAR 2005  
 COPYRIGHT (C) 2005 Merck & Co., Inc., Whitehouse Station, New Jersey, USA. All Rights Reserved.

FILE COVERS FROM LATE 19TH CENTURY TO PRESENT. LAST UPDATE: AUGUST 2004

THE MERCK INDEX ONLINE is a service mark of Merck & Co., Inc., Whitehouse Station, NJ, USA and is registered in the United States Patent and Trademark Office.

=> s L15

```

1748 B
      (BETA)
      9 CARBOLIN?
      5 B(W) CARBOLIN?
      47 PYRIDO
      148 INDOL?
      14 PYRIDO(4A) INDOL?
      15 RAUWOLFIA
      0 NORHARMANE
      2 "HYDROXAMIC"
4561 "ACID"
1106 "ACIDS"
5075 "ACID"
      ("ACID" OR "ACIDS")
      2 "HYDROXAMIC ACID"
      ("HYDROXAMIC" (W) "ACID")
      60 CARBOXAMIDE
      316 "CARBOXYLIC"
4561 "ACID"
1106 "ACIDS"
5075 "ACID"
      ("ACID" OR "ACIDS")
      313 "CARBOXYLIC ACID"
      ("CARBOXYLIC" (W) "ACID")
1058 HYDROXY
      60 AMIDE
      8 AMIDES
      67 AMIDE
      (AMIDE OR AMIDES)
      0 "CARBOXYLIC ACID" (4A) HYDROXY (3A) AMIDE
L24      0 L10 AND L14

```

=> fil medline

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
----------------------	------------------	---------------

FULL ESTIMATED COST	0.31	1743.24
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-28.93

FILE 'MEDLINE' ENTERED AT 17:28:25 ON 14 MAR 2005

FILE LAST UPDATED: 12 MAR 2005 (20050312/UP). FILE COVERS 1950 TO DATE.

On December 19, 2004, the 2005 MeSH terms were loaded.

The MEDLINE reload for 2005 is now available. For details enter HELP RLOAD at an arrow prompt (=>). See also:

<http://www.nlm.nih.gov/mesh/>  
[http://www.nlm.nih.gov/pubs/techbull/nd04/nd04\\_mesh.html](http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html)

OLDMEDLINE now back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2005 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L15

```

508219 BETA
  526 BETAS
508318 B
      (BETA OR BETAS)
  3274 CARBOLIN?
  1935 B(W) CARBOLIN?
  1487 PYRIDO
  38362 INDOL?
    530 PYRIDO(4A) INDOL?
  2389 RAUWOLFIA
    7 RAUWOLFIAS
  2389 RAUWOLFIA
      (RAUWOLFIA OR RAUWOLFIAS)
    42 NORHARMANE
  3820 "HYDROXAMIC"
1318154 "ACID"
  487203 "ACIDS"
1521924 "ACID"
      ("ACID" OR "ACIDS")
  3802 "HYDROXAMIC ACID"
      ("HYDROXAMIC" (W) "ACID")
  3792 CARBOXAMIDE
  414 CARBOXAMIDES
  4051 CARBOXAMIDE
      (CARBOXAMIDE OR CARBOXAMIDES)
  23656 "CARBOXYLIC"
    1 "CARBOXYLICS"
  23657 "CARBOXYLIC"
      ("CARBOXYLIC" OR "CARBOXYLICS")
1318154 "ACID"
  487203 "ACIDS"
1521924 "ACID"
      ("ACID" OR "ACIDS")
  17256 "CARBOXYLIC ACID"
      ("CARBOXYLIC" (W) "ACID")
  59210 HYDROXY

```

acid amides.  
AUTHOR: Lippke K P; Muller W E; Schunack W G  
SOURCE: Journal of pharmaceutical sciences, (1985 Jun) 74 (6)  
676-80.  
Journal code: 2985195R. ISSN: 0022-3549.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 198509  
ENTRY DATE: Entered STN: 19900320  
Last Updated on STN: 19970203  
Entered Medline: 19850925

AB Numerous **beta-carboline-3-carboxamides** were synthesized by amidation of **beta-carboline-3-carboxylic acid**, with various amino acids and amino acid esters serving as amine components, and tested in respect to their affinity for the benzodiazepine receptor in mouse brain membranes. The title compounds have affinities in the low micromolar range. The results are discussed with respect to their relevance for a possible **beta-carboline** structure containing the endogenous ligand of the benzodiazepine receptor.

L25 ANSWER 64 OF 70 MEDLINE on STN  
ACCESSION NUMBER: 85237091 MEDLINE  
DOCUMENT NUMBER: PubMed ID: 2989508  
TITLE: Supraspinal convulsions induced by inverse benzodiazepine agonists in rabbits.  
AUTHOR: Massotti M; Lucantoni D; Caporali M G; Mele L; Gatta F  
SOURCE: Journal of pharmacology and experimental therapeutics, (1985 Jul) 234 (1) 274-9.  
Journal code: 0376362. ISSN: 0022-3565.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 198508  
ENTRY DATE: Entered STN: 19900320  
Last Updated on STN: 19900320  
Entered Medline: 19850820

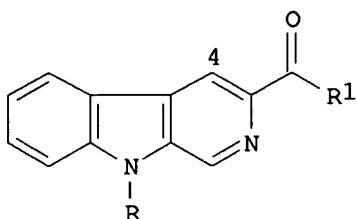
AB The electroencephalographic (EEG) effects of inverse benzodiazepine (BDZ) agonists have been studied in rabbits after i.v. administration. A dose-dependent progression of three different stages of EEG changes have been observed with inverse BDZ agonists. At first, trains of slow waves in the occipital cortex occur, followed by trains of spike-and-wave complexes in the sensorimotor cortex. These two stages are superimposed on a desynchronized cortical activity, accompanied by an enhancement of the hippocampal theta rhythm. These EEG changes parallel a state of alertness. The third stage is characterized by generalized grand-mal seizures made up of high voltage spikes in the cortical and subcortical brain areas accompanied by generalized tonico-clonic convulsions. No modification of electrical activity is observed at the level of the spinal cord. Methyl-**beta-carboline-3-carboxylate** (beta-CCM) (at doses higher than 0.2 mg/kg) and 6,7-dimethoxy-4-ethyl-**beta-carboline-3-carboxylate** (DMCM) (at doses higher than 0.4 mg/kg) elicit all three stages, whereas ethyl-**beta-carboline-3-carboxylate** (beta-CCE) (0.2-2 mg/kg) and N-methyl-**beta-carboline-3-carboxamide** (2-20 mg/kg) only elicit the first two, and finally CGS 8216 only the first. The extent of the EEG progression by inverse BDZ agonists may therefore be used as an index of the efficacy of each compound. The BDZ antagonists Ro 15-1788 and Ro 15-3505 (0.3 mg/kg or higher), which do not change the EEG pattern, block the effects of the convulsant and subconvulsant doses of the inverse BDZ

L15 ANSWER 66 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1996:110120 CAPLUS  
DOCUMENT NUMBER: 124:193312  
TITLE: In vivo potent antifilarial  $\beta$  -  
**carbolines**  
AUTHOR(S): Agarwal, Alka; Agarwal, Shiv K.; Singh, Som Nath;  
Fatma, Nigar; Chatterjee, R. K.  
CORPORATE SOURCE: Div. Med. Chem., Central Drug Res. Inst., Lucknow,  
226001, India  
SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(3),  
225-8  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB 1-Methoxycarbonyl/carboxamido/cyano-9H-pyrido[3,4-b]  
**indoles** have been found to exhibit interesting in vivo filaricidal  
activity against Litomosoides carinii and Acanthocheilonema viteae in  
rodents.

L15 ANSWER 67 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1995:940148 CAPLUS  
DOCUMENT NUMBER: 124:45456  
TITLE: Continuous exposure to FG 7142: behavioral  
sensitization is not accompanied by changes in  
benzodiazepine/GABA receptor coupling  
AUTHOR(S): Brett, R. R.; Jedrusik, P.; Laverty, W.; Pratt, J. A.  
CORPORATE SOURCE: Department Physiology and Pharmacology, University  
Strathclyde, Glasgow, G1 1XW, UK  
SOURCE: Journal of Psychopharmacology (Oxford) (1995), 9(3),  
223-7  
CODEN: JOPSEQ; ISSN: 0269-8811  
PUBLISHER: Oxford University Press  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Chronic intermittent high-dose treatment with N-methyl- $\beta$  -  
**carboline-3-carboxamide** (FG 7142) leads to kindling  
accompanied by reduction in  $\gamma$ -aminobutyric acid (GABA) receptor  
function, whereas chronic continuous administration may result in  
behavioral effects in the opposite direction from those of acute FG 7142.  
In the present study, the authors have investigated the effects of  
continuous administration of low doses of FG 7142 on the response to an  
acute challenge dose of FG 7142 in an ethol. based model of anxiety. Rats  
treated continuously for 14 days with FG 7142 delivered by osmotic  
minipump at a rate of 1.2-1.5 mg/kg/day showed sensitization to the  
anxiogenic effects of a challenge dose of FG 7142 (6 mg/kg), as measured  
in the elevated plus-maze. This was not accompanied by any change in  
benzodiazepine/GABA receptor coupling, as assessed by the "GABA shift".  
These results indicate that continuous low-dose treatment with FG 7142 can  
elicit sensitization to the behavioral effects of FG 7142, but that this  
is unlikely to be mediated by changes in benzodiazepine/GABA receptor  
coupling.

L15 ANSWER 68 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1995:933387 CAPLUS  
DOCUMENT NUMBER: 124:117133  
TITLE: Regioselective metalation of 9-methoxymethyl-  
**beta.-carboline-3-**  
**carboxamides** with amidomagnesium chlorides  
AUTHOR(S): Schlecker, Wolfgang; Huth, Andreas; Ottow, Eckhard;  
Mulzer, Johann  
CORPORATE SOURCE: Schering AG Berlin, Berlin, D-13353, Germany

SOURCE: Synthesis (1995), (10), 1225-7  
 CODEN: SYNTBF; ISSN: 0039-7881  
 PUBLISHER: Thieme  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 124:117133  
 GI



I

AB The N-protected  $\beta$ -carboline I (R = CH<sub>2</sub>OMe; R<sub>1</sub> = NHCMe<sub>3</sub>, NHMe) underwent exclusive metalation at C(4) with R<sub>2</sub>MgCl (R<sub>2</sub> = 2,2,6,6-tetramethylpiperidino) and/or Et<sub>2</sub>NMgCl, whereas the unprotected  $\beta$ -carboline I (R = H; R<sub>1</sub> = NHMe) was inert under these conditions. The C(4) metalated species reacted with electrophiles to give 3,4-disubstituted  $\beta$ -carboline, which are interesting precursors to physiol. active compds.

L15 ANSWER 69 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:887311 CAPLUS

DOCUMENT NUMBER: 123:295127

TITLE: N-Methyl- $\beta$ -carboline-3-carboxamide (FG 7142), an anxiogenic agent in airborne particles and cigarette smoke-polluted indoor air

AUTHOR(S): Yuan, Juan; Manabe, Shigeo

CORPORATE SOURCE: Dep. Hygiene, Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Environmental Pollution (1995), 90(3), 349-55

CODEN: ENPOEK; ISSN: 0269-7491

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB  $\beta$ -Carboline-3-carboxylic acid methylamide (FG 7142), an anxiogenic agent, has been measured in airborne particles, automobile-exhaust particles, incinerator ash, smoke condensate of tree leaves and cigarette-smoke-polluted indoor air by high-performance liquid chromatog. This compound has been detected in indoor as well as outdoor air. The source of this compound in indoor air was determined as cigarette smoke, identified from smoking machine studies. This anxiogenic agent was detected in smoke condensate of tree leaves and incinerator ash from garbage burning plants, but not in diesel-exhaust particles. Considering the present results, together with the previous finding that cigarette smoke contains this compound, FG 7142 is likely to be formed through combustion of plants. Our data also suggest that this compound may be widely distributed in the environment.

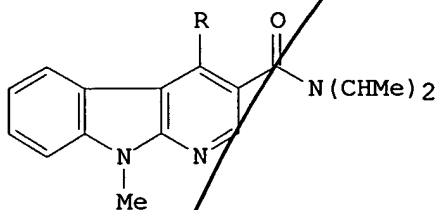
L15 ANSWER 70 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:795473 CAPLUS

DOCUMENT NUMBER: 123:306611

TITLE: Cholecystokinin antagonists containing  $\beta$ -carboline

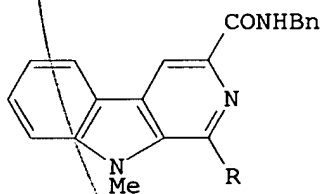
INVENTOR(S): Yamada, Koichiro; Hikoda, Masakatsu; Yura, Takeshi; Kano, Toshiaki; Nagasaki, Masaaki



I

AB The preparation of new 3-substituted  $\alpha$ -carboline (1H- **pyrido** [2,3-b]**indole** derivs.) was described and these products were subjected to ortho-lithiation expts. 3-Pivalamido and 3-carboxamido derivs. are cleanly lithiated at 4-position. The results are correlated with MNDO calcns. Various 3,4-disubstituted  $\alpha$ -carboline are obtained in excellent yields. Thus, 9-methyl-N,N-diisopropyl-1H-**pyrido**[2,3-b]**indole**-3-**carboxamide**-I(R=H)-was treated with lithium 2,2,6,6-tetramethylpiperidine and quenched with Et formate to give I (R = CO<sub>2</sub>Et) in 72% yield.

L15 ANSWER 79 OF 149 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:77199 CAPLUS  
 DOCUMENT NUMBER: 120:77199  
 TITLE: Ortho-directed lithiation studies of 3-carboxy-.  
**beta**.-carboline: a direct route to  
 4-substituted derivatives  
 AUTHOR(S): Mehta, Anita; Dodd, Robert H.  
 CORPORATE SOURCE: Inst. Chim. Subst. Nat., Cent. Natl. Rech. Sci.,  
 Gif-sur-Yvette, 91198, Fr.  
 SOURCE: Journal of Organic Chemistry (1993), 58(26), 7587-90  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

AB 9-N-methyl-3-N-benzyl- $\beta$  -carboline-3-**carboxamide** (I; R = H) was regioselectively lithiated at the C-4 position using sec-butyllithium in THF at -78°C. The anion reacted with deuterium oxide to give the corresponding 4-deuterated derivative of I (R = H) in 45% yield. A side reaction in the latter case included nucleophilic addition of sec-butyllithium to the C-1 position of the **beta**.-carboline to give compound I (R = CHMeEt). This type of side product was not formed when methyllithium instead of sec-butyllithium was used to generate the anion of I (R = H). Under these conditions, specific C-4 substitution of  $\beta$  -carboline I (R = H) was achieved in high yields using anisaldehyde, benzophenone, N,N-dimethylformamide, and Pr iodide as electrophiles. This represents the first example of the use of ortho-directed metalation in the  $\beta$  -carboline series and allows direct entry to 4-substituted 3-carboxy-.**beta**